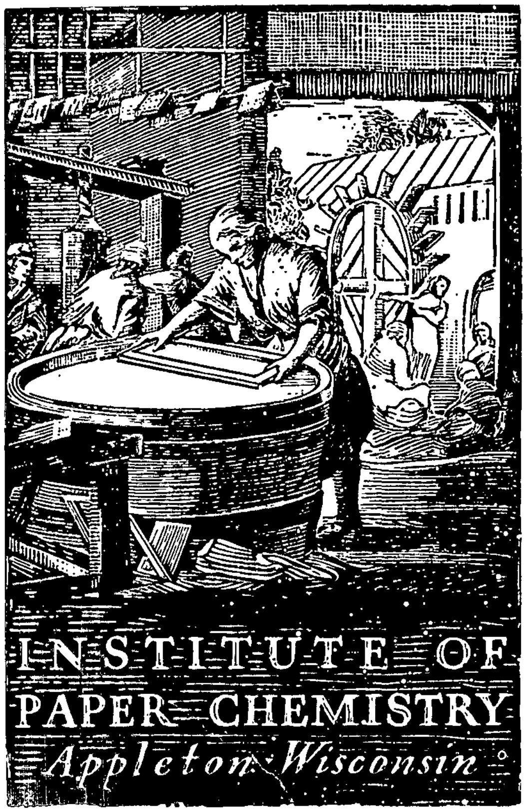

ENVIRONMENTAL SYSTEMS SIMULATION

Project 3433

Report One
A Progress Report
to
MEMBERS OF THE INSTITUTE OF PAPER CHEMISTRY

March 20, 1981

THE INSTITUTE OF PAPER CHEMISTRY

Appleton, Wisconsin

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SUMMARY

Process simulation is an important tool for evaluating alternative strategies which minimize process effluents. DYSCO, a dynamic, sequential, modular process simulator has been modified for use in the pulp and paper industry.

DYSCO was used to model both the steady state and dynamic behavior of the water system of a fine paper machine. The initial response of the water system to a web break was simulated and the results indicated that the saveall experiences a rapidly fluctuating load.

The "TAPPI benchmark problem" was studied with DYSCO. This problem was intended to be used to study various steady state simulators, but was easily simulated with DYSCO. The steady state results agreed with the published results (9).

A dynamic model of an activated sludge reactor was developed and included in the process model library. This model tracks the behavior of two types of organisms and a variety of other components. The model was compared to laboratory data, but has not been verified by comparing it to a full scale activated sludge system.

INTRODUCTION

Historically, the pulp and paper industry has been a large user of water. Unlike most industries in which 10-20% of the intake water is used in the process, the pulp and paper industry uses nearly 60% of its intake water as process water (1). Thus, this industry faced a major, massive problem when process effluents were required to be biologically treated.

Efforts to reduce water consumption have been going on for many years. Water system closure leads to many design and operating questions. First and foremost among these questions is the impact such closure will have on the manufacturing process. System closure leads to a buildup of chemicals and fiber fractions. Special care must be taken to ensure that this buildup remains below critical levels. The temperature of the water system also increases. Again, care must be taken to ensure that such temperature increases stay within the bounds of safe operating conditions.

Another, less obvious, effect is the impact such system closure may have on the waste treatment plant. The waste treatment plant is designed to treat a given range of effluent flows with a given set of characteristics. As with any process, the treatment facility can accept a range of influent characteristics, but variations must not be too large or extend over too long a period of time. As the mill water system is closed, the mill sewer flows are, on the average, reduced but become more concentrated. Accidental spills and washings from various clean up operations can then contribute significant volumes to the mill sewers. These intermittent discharges can cause rapid, wide fluctuations in treatment plant influent quality and quantity. If the fluctuations are too wide or too rapid, the biological reactor may be upset and take many days to return to normal operating levels. The cost of discharging an effluent which does not meet state or federal permit levels may be very expensive. Thus, proper measures must be taken to ensure that such occurrences are minimized.

The impact of water system closure can be estimated through simulation of the process. The changes in process stream characteristics can be estimated by modelling the process and the impact of such changes are determined by experts on various portions of the process; our knowledge of the process is not good enough to allow such things as increased corrosion rates or changes in retention to be explicitly modelled. Spill control plans and process control schemes can also be simulated.

SIMULATION EFFORT

Several years ago we recognized the need to develop the capability to simulate various portions of the process. The need to follow time varying events required a dynamic simulation capability. Reports on Project 3251 - White Water Recycle Simulation (2,3) describe that early work. This report is essentially a continuation of that effort and covers three main topics.

I. First, there will be a brief discussion of the simulator, DYSCO. While the development work is ongoing, the major portion of it is complete and the program is now available to our member companies at a nominal fee.

II. Secondly, the use of the simulator to model papermaking processes will be covered. This modelling activity includes steady state results of water system closure and a study of the water system during a web break.

Recently a group has been formed within TAPPI to investigate the industry needs and status vis-a-vis process simulation. To aid in the comparison of various simulators, a standard, or benchmark, problem was developed. This problem was designed to test steady state simulators. While DYSCO is not only a steady state simulator, it can solve steady state problems. Therefore, we obtained a copy of the TAPPI benchmark problem and simulated it using DYSCO. The problem and the results will be briefly discussed.

III. The third main topic will be a somewhat detailed discussion of our initial efforts in developing a waste water treatment plant model. For this work, we chose to model the activated sludge process and used, as a starting point, the model developed by Busby (4).

I. DYSCO - AN INTERACTIVE EXECUTIVE FOR THE DYNAMIC SIMULATION AND CONTROL OF CHEMICAL PROCESSES

THE SIMULATOR

DYSCO is a dynamic, modular, sequential simulator. It was originally developed for use in the petrochemical industry (5). Extensive additions and revisions have been made over the last several years at The Institute of Paper Chemistry to tailor the program to meet the needs of the pulp and paper industry. With a few minor exceptions, the entire program is written in FORTRAN IV, so it can be run on most large computers.

The basic premise behind DYSCO is that the process to be simulated can be broken into a set of subprocesses, or unit operations. These unit operations are connected to each other by flows of material, energy, or information and are shown as streams or pipes. DYSCO consists of an executive program for handling the information flow (be it material, energy or control signals) between the basic process units, a library of process models from which the user builds a representation of the desired process, and a set of computer routines and data files that are necessary to compute thermo-physical properties of the streams.

DYSCO is a two part simulator, with each part (or phase) a separate, standalone program. The first part (DYSCO1) interactively requests the user to supply the process flowsheet (topology) and the number of components, or compounds, that are in the process fluids. These compounds are conventionally called stream components. DYSCO1 takes this information, reorganizes it and checks it for consistency. The user is informed of any potential errors, such as the use of duplicate stream numbers, missing stream numbers, etc. and the user is allowed to correct such errors. The process topology is then written to a file for later use by the second phase of DYSCO (DYSCO2). DYSCO1 also produces two FORTRAN routines which must be linked to DYSCO2. The purpose of these routines is to minimize computer memory use by defining arrays only as big as needed by the problem and to ensure that only the required process models are included in the simulation.

Phase 2, or DYSCO2, is the main simulation phase of DYSCO. It obtains the process topology that was set up by DYSCO1 and then interactively requests design information about each unit. That is, it requests parameters such as the volume of tanks and the relative splits around a distribution manifold. Stream data are also requested from the user. He must initialize the process input streams, but may also initialize other pipes. Assorted control information must be supplied by the user.

When using DYSCO to obtain dynamic results, four numerical integration techniques are available. Euler's method is the one most often used for initial testing and the variable step Adams-Moulten predictor-corrector algorithm is used for production runs. A fourth order Runge-Kutta method and a variable step, fourth order Runge-Kutta method are also available. When using the variable step methods, the user has control over the error criteria used for changing the time step and how often this error condition is checked.

The basic function of all process models in the DYSCO library is to transform input streams into output streams. Dynamic models first compute the time rate of change of the appropriate process variables. These derivative values are used by the selected integrator to compute updated values. Steady state models simply transfer the inputs into outputs. This type of structure allows DYSCO to be a steady state simulator as well as a dynamic process simulator. If the simulated process contains no dynamic elements, a converged solution is reached by the process of successive substitutions. A steady state simulation may also be terminated after a fixed number of iterations. If dynamic elements are used, the simulation runs for a specified amount of time. That is, the user starts the simulation at time zero, and specifies the upper limit, be it an hour, a day, a month, etc. During a dynamic simulation, a user specified set of stream components is checked for steady state levels after each iteration. If the test is true, the simulation may, at the user's discretion, be terminated.

Table I is a list of the process models currently available in DYSCO. Of these, only the TANK and ACTSLG models are dynamic. The remainder are simple steady state models. However, the TANK model, coupled with the CONTRL and VALVE models allows a great variety of dynamic processes to be simulated. FGEN, plus the ability to impose step and ramp functions on any process variable, gives the user the ability to upset the process with a variety of disturbances.

PHYSICAL PROPERTIES

DYSCO was originally developed with the intent of using the extensive physical property data banks generated for petrochemical industry simulators. By and large, the pulp and paper industry does not need these data banks which normally consist of extensive descriptions of the thermodynamic properties of various organic compounds.

Development of a physical property data bank for use in the pulp and paper industry is a desirable and necessary addition to DYSCO if the program is to be of great utility. To date, only a limited data bank is available. It includes temperature independent heat capacities for fiber, water and TiO_2 as well as a fairly extensive set of steam tables. An attempt has been made to include some retention data, but the data have not been verified. Nevertheless, the necessary routines to access the physical property data bank are present and the data bank can be expanded as required.

TABLE I

DYSCO MODULES

ACTSLG	- Mixes N influent streams and treats the biodegradable components in a biological reactor. The reactor can be populated by two species of bacteria.
ADDFLO	- Takes one stream and adds material from a second stream to raise the first stream to a desired flow rate.
AFLASH	- Performs an adiabatic, pure component flash on a stream.
CLEANR	- Takes one input stream and produces an accept and reject stream. A percentage of each component from the input stream is calculated by a standard cleaner function and put in the reject stream.
CONCNT	- The first output stream contains a specified percentage of a specified component at a specified mass fraction from the input stream.
CONTRL	- Models a general proportional, integral, and derivative controller. CONTRL handles information streams only and is designed to be used in conjunction with VALVE.
CONVAL	- Controls the flow out of a MIXER at a constant rate.
DILUTR	- Takes one input stream and dilutes a specified component or components with a second input stream to a specified consistency.
FGEN	- A function generator. FGEN will change a stream or unit parameter according to a specified function (SIN, COS, EXP).
HEADER	- Takes the flow from one output stream and splits it into any number of output streams according to specified percentages.
HEATER	- Mixes several input streams together, then adds a specific amount of heat or changes the temperature.
MIXPNT	- Takes any number of input streams and adds them together to form an output stream.
REFINR	- Converts a portion of each of the components except one designated component into that designated component according to a typical refiner function. REFINR also adds heat per unit of mass to the stream.
REGLTR	- Splits one stream into two, the first of which has a user designated flow and the second, the excess from the input stream.

TABLE I (continued)

DYSCO MODULES

SAVALL	-	Models a typical disk saveall. It takes one input stream and divides it into three output streams (clear and cloudy filtrate and a cake stream). The user specifies the consistencies of the clear and cloudy streams, the percentage of the input water in these two streams combined, and the ratio of water in the clear stream to the water in the cloudy stream.
SCREEN	-	Takes a specified percentage of each component from an input stream and puts it in an output stream. The difference is put in a second output stream.
TANK	-	A dynamic MIXPNT. TANK has a volume.
VALVE	-	Models a parabolic control valve with direct or inverse action.
VSPLIT	-	Splits one input into two outputs based upon a signal from a controller (CONTRL)

II. APPLICATION OF DYSCO IN PAPERMAKING PROCESSES

Several problems have been used to test DYSCO. Such problems serve to test the simulator code for correctness as well as to demonstrate the utility of the simulator. The two problems that will be discussed are basically paper machine area problems, although DYSCO has been used to simulate a groundwood mill (2), a CEDED bleach plant (6), and another paper machine (7).

PAPER MACHINE TEST PROBLEM

The first major test problem was the simulation of a complete paper machine water system. Only the material balance was of concern; the energy balance was not done.

The paper machine chosen for this study was a relatively modern, fine paper machine producing about 250 tons per day. This machine had previously been modelled using a version of the GEMS (8) program. Thus a detailed schematic and extensive data base already existed and eliminated the need to measure the necessary data. The necessary parameters for the model were easily calculated from these data.

Simulation of this paper machine included five simulation runs. First, a base case was simulated, followed by three water system closure studies (options 1-3). These four runs were done to determine the steady state flows and concentrations of fiber and clay in each system. The fifth run (option 4) evaluated the dynamic response of the system to a web break. A diagram of the paper machine is shown in Fig. 1. A description of the process and the results for each of these five runs follows.

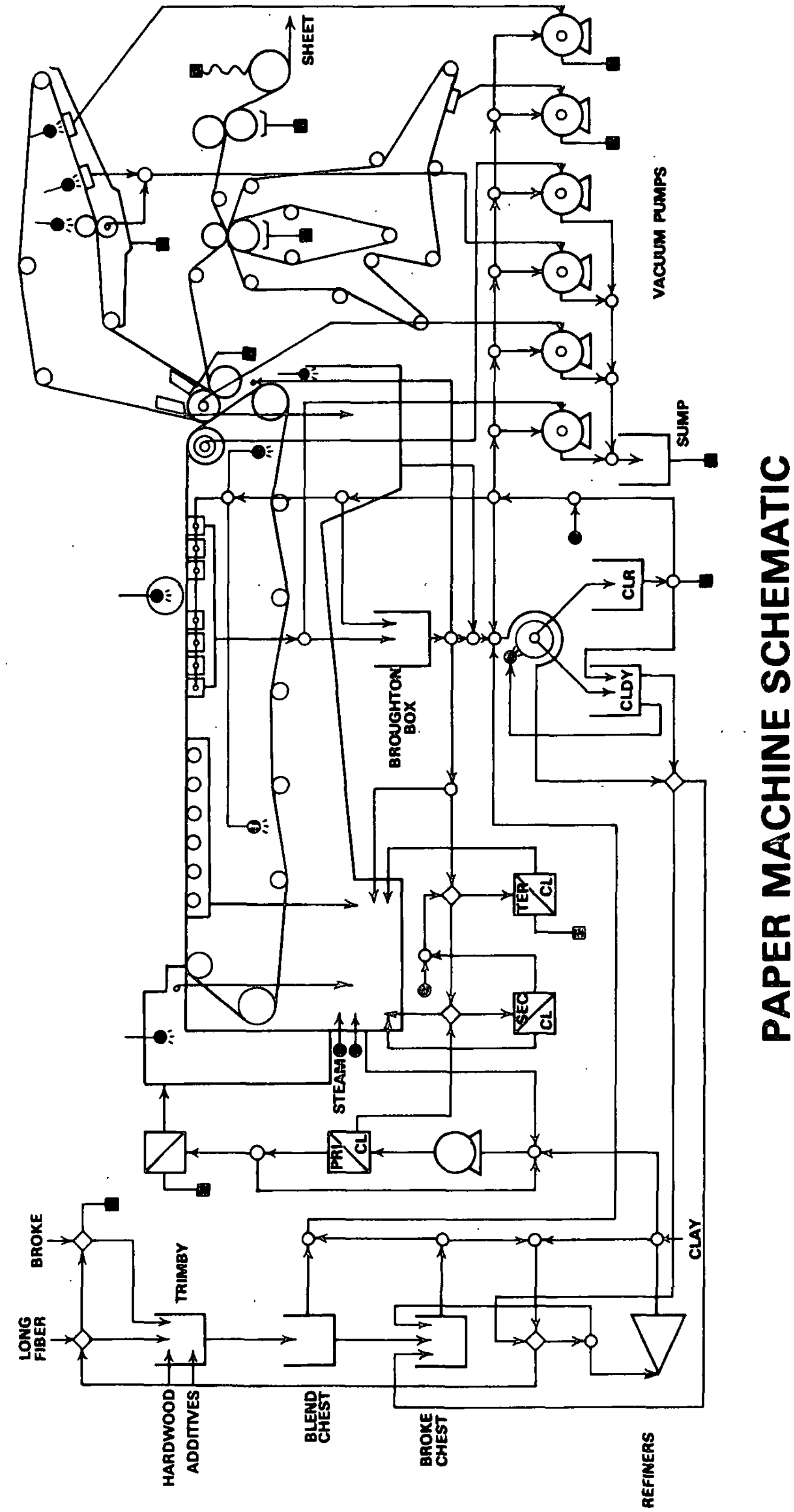

Figure 1. Paper Machine Schematic

SIMULATION RUN 1 - BASE CASE

Inputs

The total fiber input to the system was 303 lb/minute which included hardwood kraft, long fiber and broke. TiO_2 and other additives were combined into one category entitled 'filler' and added to the system at the rate of 39.2 lb/minute. Water entered the system at the rate of 1060 gpm. This included stock dilution water, showers, steam, clear filtrate make-up and additive made-down. Table II summarizes all of the inputs for the base case.

Outputs

The sheet left the dryer section at the rate of 346 lb/minute with a moisture ratio of 0.047 (moisture ratio = lb water/lb bone dry fiber). This included 298 pounds of fiber per minute of the 303 pounds per minute entering the system. The dryers removed 61 gallons/minute of water in the form of steam. Losses from the system were in the form of tertiary cleaner and selectifier screen rejects, vacuum pump discharges, and some press water. Small quantities of cloudy filtrate and suction box white water were also sewered.

Total loss to the sewer included 997 gpm of water, 4.78 lb/minute of fiber and 5.0 lb/minute of filler. Table III summarizes all of the outputs from the system. Figure 2 is a block diagram summarizing the important flows.

Refining, Cleaning, and Screening Systems

After leaving the machine chest, the stock is refined with Jordan refiners and clay and starch are then added. White water from the tray silo joins the stock for further dilution before the fan pump.

TABLE II

BASE CASE INPUTS

	Water, gpm	Fiber, lb/minute	Filler, lb/minute
Broke	0.34	51.3	9.67
Hardwood kraft	440.0	149.0	0.69
Long fiber	0.59	99.9	--
TiO_2	9.53	--	18.4
Rosin	10.8	1.28	--
P. Ad.	6.00	--	10.5
Alum	0.69	--	--
Dye	2.12	--	--
Starch	10.0	2.06	--
Steam	7.86	--	--
Make-up at tray silo	52.9	--	--
Cleaners	0.70	--	--
Headbox shower	16.2	--	--
Dandy shower	9.93	--	--
Clear chest make-up	331.0	--	--
Uhle box wetting shower	17.0	--	--
Dilution at couch pit	57.4	--	--
Felt showers	88.0	--	--
Total	1061.0	303.0	39.2

TABLE III

BASE CASE OUTPUTS

Vacuum Pumps	Water, gpm	Fiber, lb/minute	Filler, lb/minute
Uhle box	65.7	0.031	0.043
Suction box	63.3	0.270	0.434
Couch	539.0	1.41	0.930
Suction pick-up	70.7	0.916	1.88
Wringer	95.0	0.116	0.177
Felt conditioning	116.0	0.045	0.353
SUB TOTAL	950.0	2.79	3.82
Tertiary rejects	23.9	1.71	0.748
Selectifier screen rejects	0.81	0.039	0.019
Excess cloudy filtrate	4.49	0.005	0.003
Excess dilution water at couch pit	0.18	0.002	0.002
Press pan sewer	17.5	0.240	0.428
TOTAL EFFLUENT	997.0	4.78	5.02
Steam from dryers	61.0	--	--
Product	1.68	298.0	34.1
TOTAL OUTPUTS	1060.0	303.0	39.1

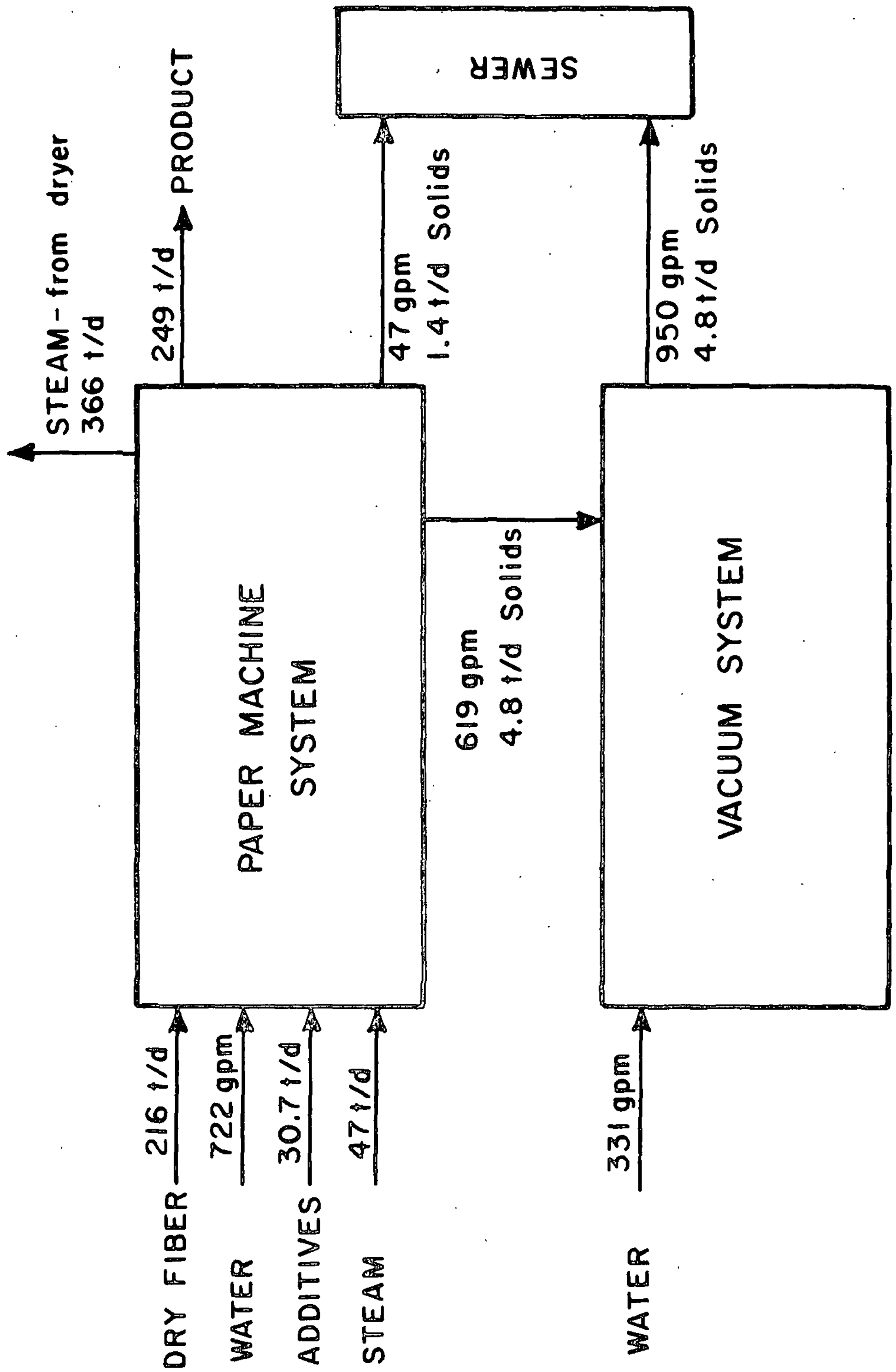

Figure 2. Base Case Flows

The fan pump feeds a conventional three stage cyclone cleaning system at the rate of 10,800 gpm. The accepts from the primary cleaner go to the selectifier screen. Secondary and tertiary accepts go to the tray silo. As seen in Table III, the tertiary rejects are sewered at the rate of 23.9 gpm of water, 1.71 lb/minute of fiber and 0.748 lb/minute of filler. Rejects from the selectifier screen are sewered at the rate of 0.81 gpm of water, 0.039 lb/minute of fiber and 0.019 lb/minute of filler. Table IV gives the efficiency of each of these screens.

TABLE IV

CLEANER EFFICIENCIES

	Input Flow, gpm	Consistency	Efficiency[a] Water, %	Fiber, %	Filler, %
Primary cleaner	10,800	6.60×10^{-3}	10.0	14.9	16.5
Secondary cleaner	1,510	7.10×10^{-3}	8.5	8.0	10.8
Tertiary cleaner	186	4.91×10^{-3}	12.9	22.4	13.6
Overall cleaner system	926	3.5×10^{-3}	0.26	0.003	0.004
Bird centriscreens	8,180	6.3×10^{-3}	0.01	0.009	0.012
Overall system	926	3.5×10^{-3}	0.269	0.340	0.384

[a]Efficiency is the ratio of reject flows to input flows.

Fourdrinier System

The fourdrinier system includes table rolls, suction boxes, and a couch roll. The moisture ratio of the sheet as it leaves the slice is 158. The tray silo collects white water from the table rolls along with the cheek bleed, secondary and tertiary accepts and wire return shower water. This white water at a consistency of 0.27% is used for stock dilution prior to the fan pump. The moisture ratio of the sheet after the table rolls is reduced to 60.

The suction boxes extract 2,240 gpm of white water at 0.1% consistency which reduces the sheet moisture ratio to 5.1. The Broughton box collects this water, directs the amount needed for dilution to the cleaners and sends the balance to the saveall.

The couch vacuum pump extracts and sewers 57.8 gpm of white water at 0.26% consistency leaving the moisture ratio of the sheet at 3.6. Net fiber and filler retentions on the wire from the slice to the sheet leaving the couch roll are 74.4% and 24.6%, respectively.

Saveall System

This saveall is a Dorr-Oliver disk filter with ten disks, each 9 feet in diameter. Water from the couch pit and Broughton box feeds the saveall with sweetener coming from the blend chest and the machine chest. The total flow to the saveall is 1,639 gpm, producing approximately 1.53 gpm of filtrate/ft^2 of filter area. Of the filtrate, approximately 47% is clear filtrate and 53% is cloudy filtrate. The resultant cake is diluted, repulped, and recycled to the machine chest. The cloudy filtrate is used as dilution water for the cake repulper, the refiners, and for the long fiber. The clear filtrate is used for trim knock-off showers, wire return showers, felt showers and vacuum pump seals. Water (4.49 gpm) is sewered as cloudy filtrate along with 0.005 lb/minute of fiber and 0.003 lb/minute of filler. There is no excess clear filtrate.

Vacuum Pump System

Vacuum pumps are used on the wire suction boxes, the couch roll, the pick-up roll, wringer press, Uhle box, and felt suction boxes. Clear filtrate made up with fresh water is used for seals on the vacuum pumps and then sewered. Also sewered is the white water extracted by each of the vacuum pumps with the exception of 2,210 gpm of the white water from the wire suction boxes which goes to the Broughton box. The total sewer loss from the pumps amounts to 950 gpm of water, 2.79 lb/minute of fiber and 3.28 lb/minute of filler.

SIMULATION RUN 2 - REDUCE SEAL WATER USAGE ON THE COUCH VACUUM PUMP (OPTION NO. 1)

The greatest water loss to the sewer occurred at the couch vacuum pump. This pump was designed for a seal flow rate of 170 gpm but was using 482 gpm. To determine the effect of reducing the excessive seal water usage, everything in the base case was held constant with the exception of the flow in two pipes. The seal water flow was reduced to the recommended design flow which in turn allowed the fresh water make-up to the clear chest to be reduced by the same amount, 312 gpm. Simulation results concluded that total water loss to the sewers could be reduced by 31% by replacing or repairing the couch vacuum pump. All other flows throughout the system remained the same. The product and all other sewer flows remained constant.

SIMULATION RUN 3 - RECYCLE VACUUM PUMP DISCHARGES TO THE SAVEALL VAT (OPTION NO.2)

An analysis of the data showed that 95.8% of the flow, 60.8% of the fiber and 76.4% of the filler in the wet end effluent originated from the vacuum pump sewers. Existing equipment at the paper machine site included a separate pump adequate for recycling discharges from the suction box, couch, suction pick-up, and wringer press vacuum pumps to the saveall vat. The sewer flow from these four pumps was collected and recycled back through the Broughton box to the saveall. The efficiency of the saveall was changed slightly in order to retain the quality of the clear and cloudy filtrate in the base case. Relative filtrate splits, 57% through the cloudy port and 43% through the clear port, were also held the same as in the base case. No fresh water make-up was required at the clear chest and this reduced fresh water consumption by 58%.

Clear filtrate increased from 653 gpm to 1150 gpm and cloudy filtrate increased from 872 gpm to 1270 gpm. The fiber in the cake increased from 29 lb/minute to 176 lb/minute. Of this 147 pound increase, 62 pounds were added sweetener from the blend chest. The extra 501 gpm of clear filtrate made it possible to eliminate the entire fresh water make-up at the clear chest. In the base case, 4 gpm of cloudy filtrate were in excess of process needs and were sewered. This option produced an extra 398 gpm of cloudy filtrate at the cloudy port. The larger cake demanded more cloudy dilution water but 226 gpm of cloudy filtrate were still in excess of process needs and had to be sewered.

As was mentioned previously, the saveall is producing 43% clear filtrate and 57% cloudy filtrate. If it were operating according to the manufacturer's recommendations, this split would be 70% clear and 30% cloudy. This would allow the recovery of more fiber and reduce the load on the effluent treatment system.

With this option, another problem arises at the saveall. The input flow at the saveall is now 2630 gpm which results in 2.46 gpm of filtrate/sq ft of filter area. Normally, a fine paper machine saveall should produce 1-2 gpm of filtrate/sq ft of filter area. In order to produce more than this, the saveall would have to run at higher rpm's and the quality of both filtrates would suffer.

Recycling the four vacuum pump discharges to the saveall would produce a savings of 331 gpm of fresh water and would reduce total effluent by 331 gpm of water, 1.50 lb/minute of fiber and 3.27 lb/minute of filler. Production would increase slightly from 346 to 351 lb/minute or a total of 3.86 tons per day. In order to implement this system, however, a more efficient and substantial saveall system would have to be installed.

Table V summarizes the outputs from Option No. 2, while Figure 3 shows the important flows.

TABLE V

OPTION 2 OUTPUTS

Vacuum Pumps	Water, gpm	Fiber, lb/minute	Filler, lb/minute
Uhle box	65.8	0.034	0.048
Suction box	--	--	--
Couch	--	--	--
Suction pick-up	--	--	--
Wringer	--	--	--
Felt conditioning	116.0	0.049	0.038
SUB TOTAL	182.0	0.083	0.086
Tertiary rejects	23.9	1.69	0.770
Selectifier screen rejects	0.83	0.819	0.039
Excess cloudy filtrate	226.0	0.267	0.176
Excess clear filtrate	200.0	0.069	0.017
Excess dilution water at couch pit	15.8	0.112	0.194
Press pan sewer	17.6	0.242	0.465
TOTAL EFFLUENT	666.0	3.28	1.75
Steam from dryers	61.6	--	--
Product	1.69	300.0	37.1

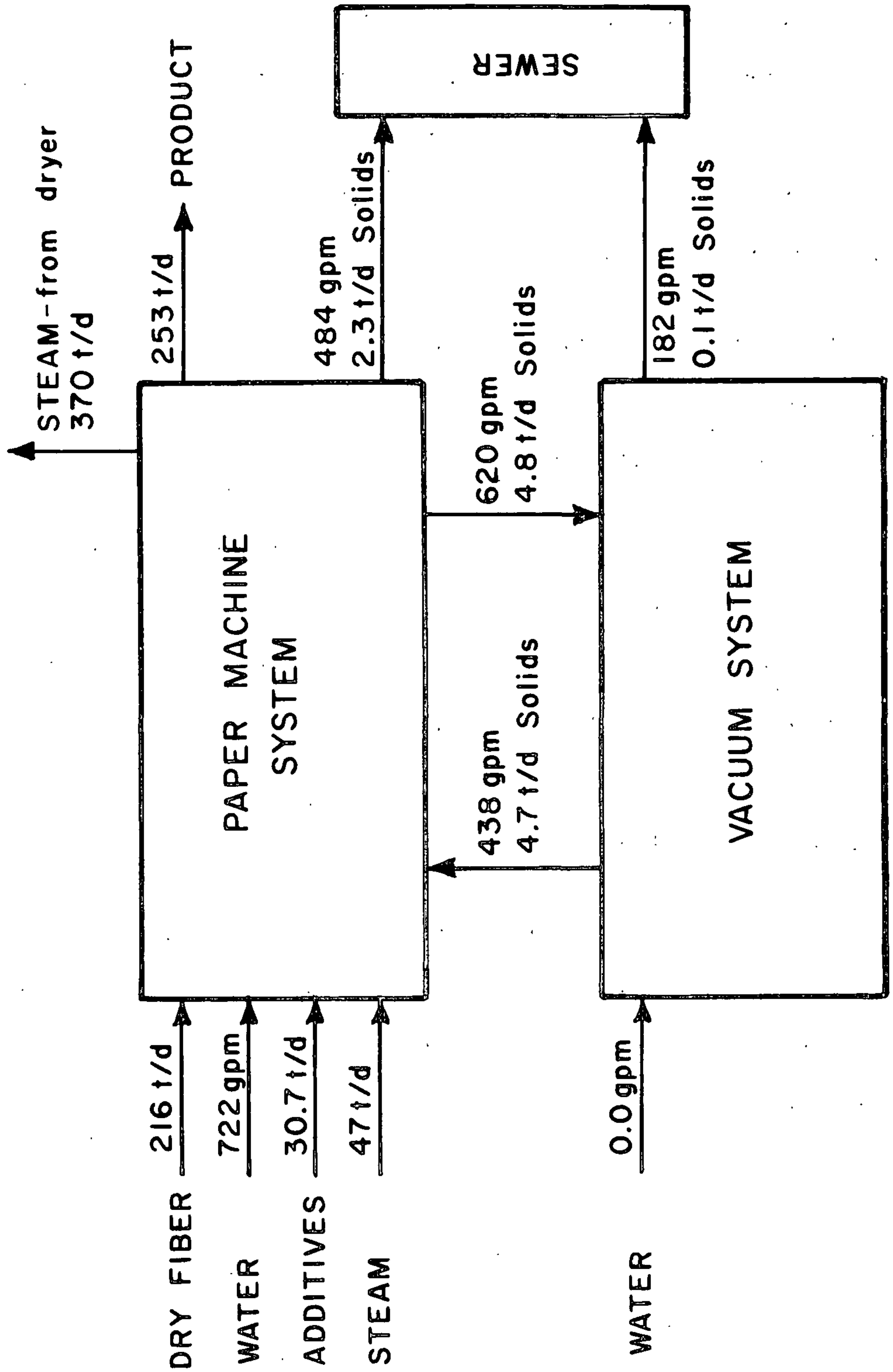

Figure 3. Option No. 2 - Flow Rates

SIMULATION RUN 4 - REVISE SAVEALL SYSTEM ALONG WITH CLEAR AND CLOUDY FILTRATE USES (OPTION NO. 3)

As mentioned in the previous option, design specifications for the filtrate percentages from the saveall are 70% clear and 30% cloudy. In the base case the split was 43% through the clear port and 57% through the cloudy port. The base case also incorrectly used cloudy filtrate upstream from the saveall. This could seriously affect wet end stability during a grade or color change. Option No. 3 repiping corrected these problems.

Correcting the saveall filtrate splits produced enough excess clear filtrate for use as broke and long fiber dilution and also enough to be substituted for fresh water on the headbox showers.

In order to implement this option, saveall modifications would have to be made. Since we were only concerned with steady state results for this option, tank volumes did not affect our simulation, but most probably the clear and cloudy tanks would have to be interchanged to more appropriately accommodate the new flows from the saveall. Present capacity of the cloudy chest is 37,000 gallons and the clear chest volume is 3,400 gallons.

Results of this option were quite favorable in that with a minimum amount of equipment changes, definite improvements could be made to the operation. In addition to losing less broke during a grade or color change, 23,000 gallons per day of fresh water would not be needed. Table VI and Fig. 4 summarize the outputs for Option No. 3.

TABLE VI

OPTION 3 OUTPUTS

Vacuum Pumps	Water, gpm	Fiber, lb/minute	Filler, lb/minute
Uhle box	65.7	0.028	0.044
Suction box	63.3	0.267	0.435
Couch	540.0	1.38	0.933
Suction pick-up	70.7	0.913	1.88
Wringer	95.0	0.112	0.177
Felt conditioning	116.0	0.041	0.354
SUB TOTAL	951.0	2.74	3.82
Tertiary rejects	23.9	2.74	3.82
Selectifier screen rejects	0.81	0.038	0.019
Excess cloudy filtrate	--	--	--
Excess clear filtrate	--	--	--
Excess dilution water at couch pit	0.24	0.0002	0.0003
Press pan sewer	17.5	0.240	0.428
TOTAL EFFLUENT	993.0	4.73	5.02
Steam from dryers	61.0	--	--
Product	1.68	298.0	34.2

SIMULATION RUN 5 - RESPONSE OF THE SYSTEM TO A WEB BREAK (OPTION NO. 4)

One of the more common upsets occurring on a paper machine is a web break in the dryer section. When this happens, the sheet must be removed from the dryers

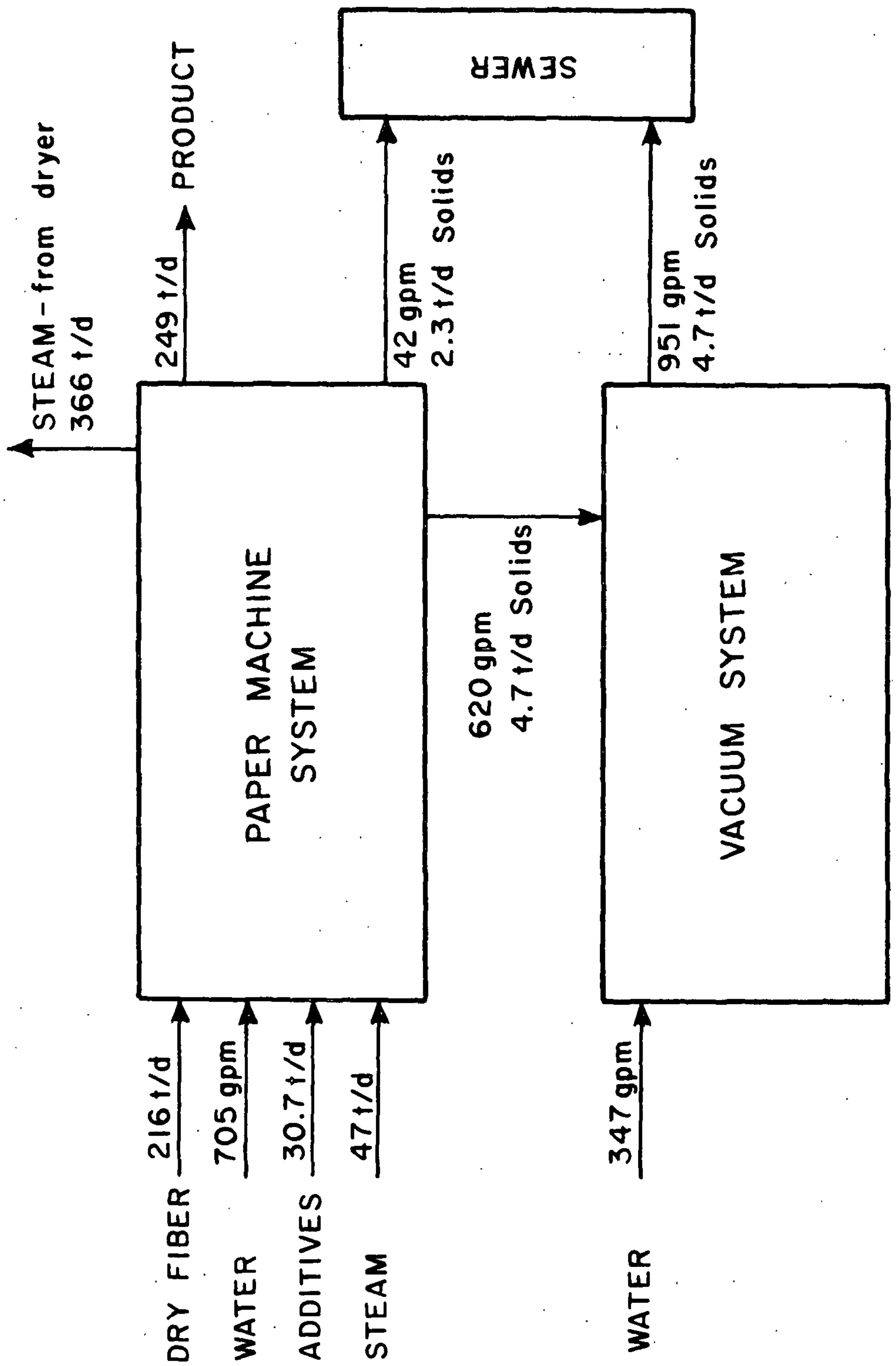

Figure 4. Option No. 3 - Flows

without shutting down the paper machine. Generally, knock off showers at the couch roll divert the sheet to the couch pit when a break is sensed. Additional dilution water is added to the couch pit and the diluted stock is returned to the stock prep system.

On this paper machine, the web break control system functions in a manner similar to the general case. When the break is sensed, the sheet is knocked into the couch pit. Broughton box water, which normally flows to the saveall, is used as additional dilution water in the saveall. It takes about 8 seconds to divert the full flow of this Broughton box water to the couch pit. A consistency controller monitors the couch pit. When the consistency rises above 3.8% (normal consistency is about 0.5%), the couch pit effluent is diverted from the saveall to the broke chest.

This control scheme causes the saveall to experience a rapidly fluctuating load. The control scheme was simulated to estimate these fluctuations. Figures 5 and 6 depict the changing fiber load to the saveall. The fiber fraction starts to rise as Broughton box water is diverted to the couch pit and the extra stock is sent to the saveall. In addition, the sweetener stock becomes a bigger portion of the flow, also increasing the fiber fraction. As evidenced in Fig. 6, the total fiber load does not initially rise, as the flow has decreased due to the hold up time in the couch pit. Eventually, this hold up causes a slight dip in the total fiber load, after 10 seconds. Rather quickly, the total fiber load to the saveall starts to rise as the sheet is sent to the saveall.

After approximately 60 seconds, the couch pit reaches the control consistency of 3.8% and the couch pit effluent is sent to the broke chest. This results in a rapid drop in saveall load (Fig. 6), but saveall vat consistency continues to rise as sweetener becomes a bigger fraction of the total flow.

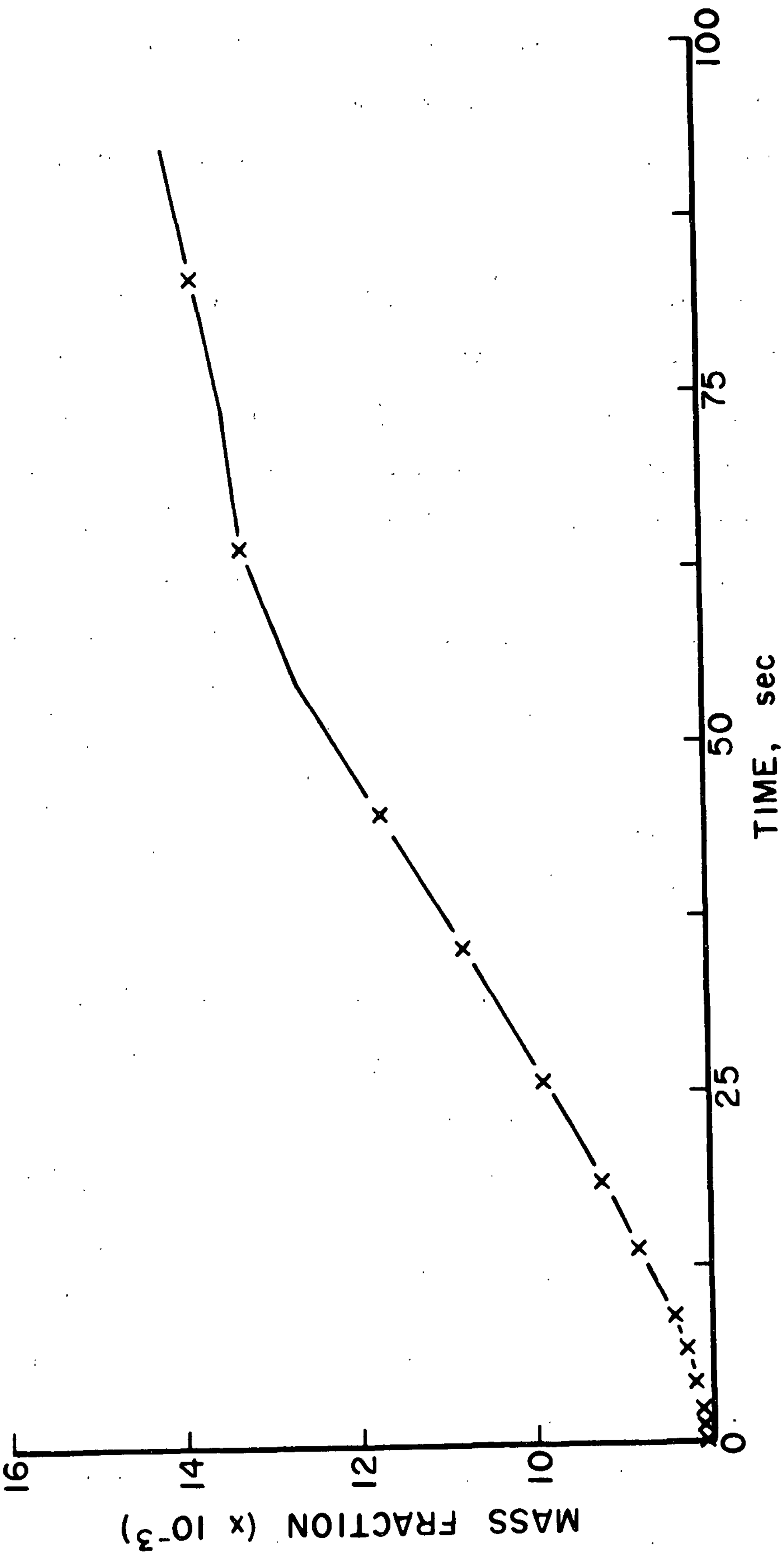

Figure 5. Option No. 4 - Fiber Fraction Input to Saveall

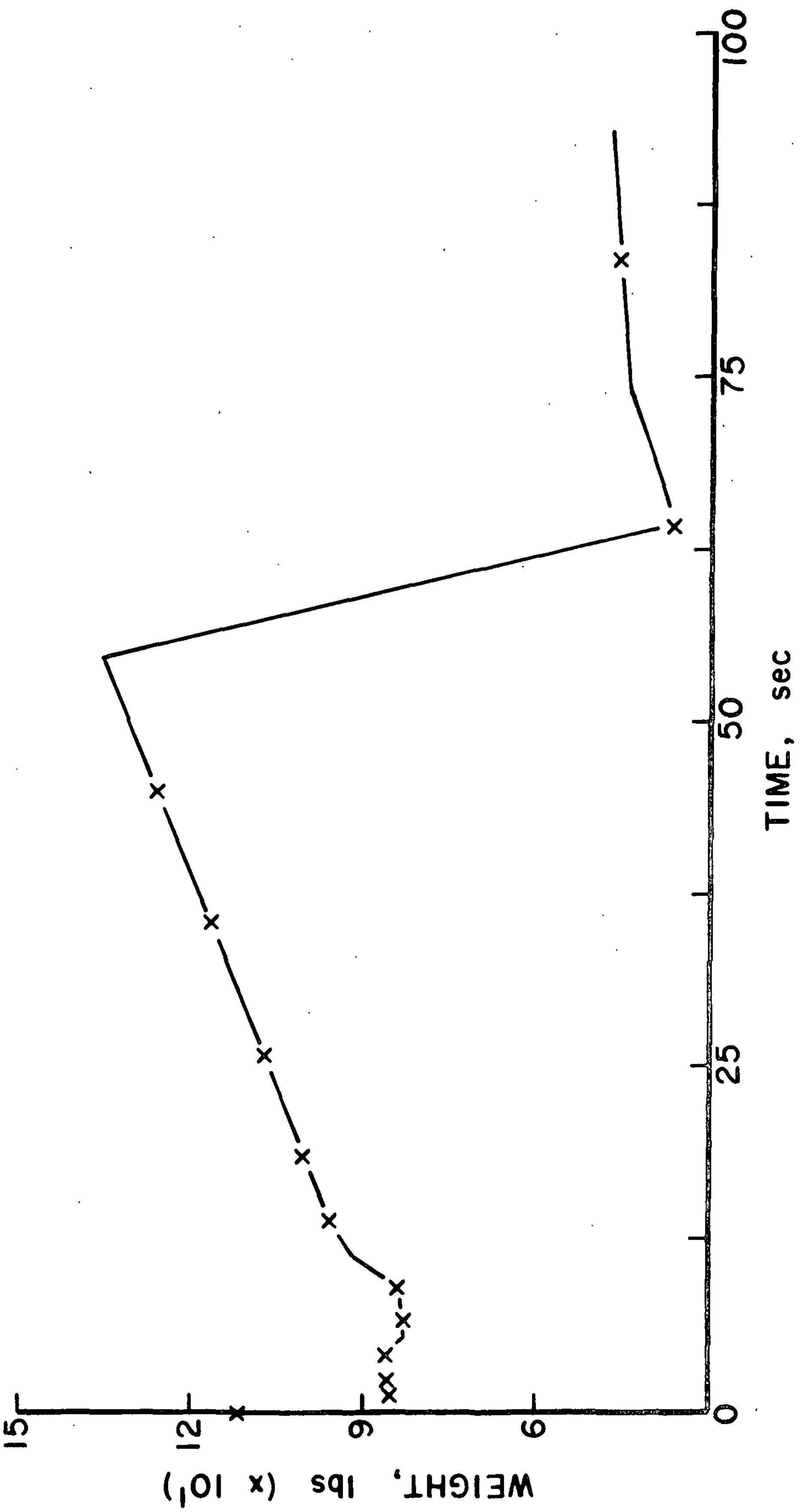

Figure 6. Option No. 4 - Fiber Load To Saveall

Filler content also changes rapidly as the web is recycled. (Recall that filler is all nonfiber material, including clay, TiO_2, alum, etc.) The simulation assumed no change in saveall characteristics as the fiber load changed. Figures 7, 8, and 9 depict the variations in the filler to fiber ratio in various saveall streams. The filler to fiber ratio drops in the saveall vat as the sheet is recycled since the sheet contains a lower filler/fiber ratio than does the normal saveall input. The cloudy filtrate stream filler/fiber ratio increases as the saveall splits a larger portion of the filler to this stream. This is a result of using constant model parameters for the saveall. In reality, the relative separation at the saveall probably changes. When the couch pit effluent is diverted from the saveall to the broke chest, the rates of change of filler to fiber also change. This is expected, as the sweetener stock, which has very little filler, becomes a more significant portion of the flow.

TAPPI BENCHMARK PROBLEM

As mentioned earlier, a group within TAPPI has recently been formed to study the simulation requirements within the pulp and paper industry. This committee is attempting to define the state-of-the-art in simulation as it is applied to the pulp and paper industry as well as to project the needs of the industry. The group is broken into four working groups:

- Evaluation of existing simulation packages
- Definition of unit operations
- Physical Property requirements
- User Requirements

This group has decided that the initial focus should be on steady state simulation packages. To aid in the comparison and evaluation procedure, a "benchmark" problem

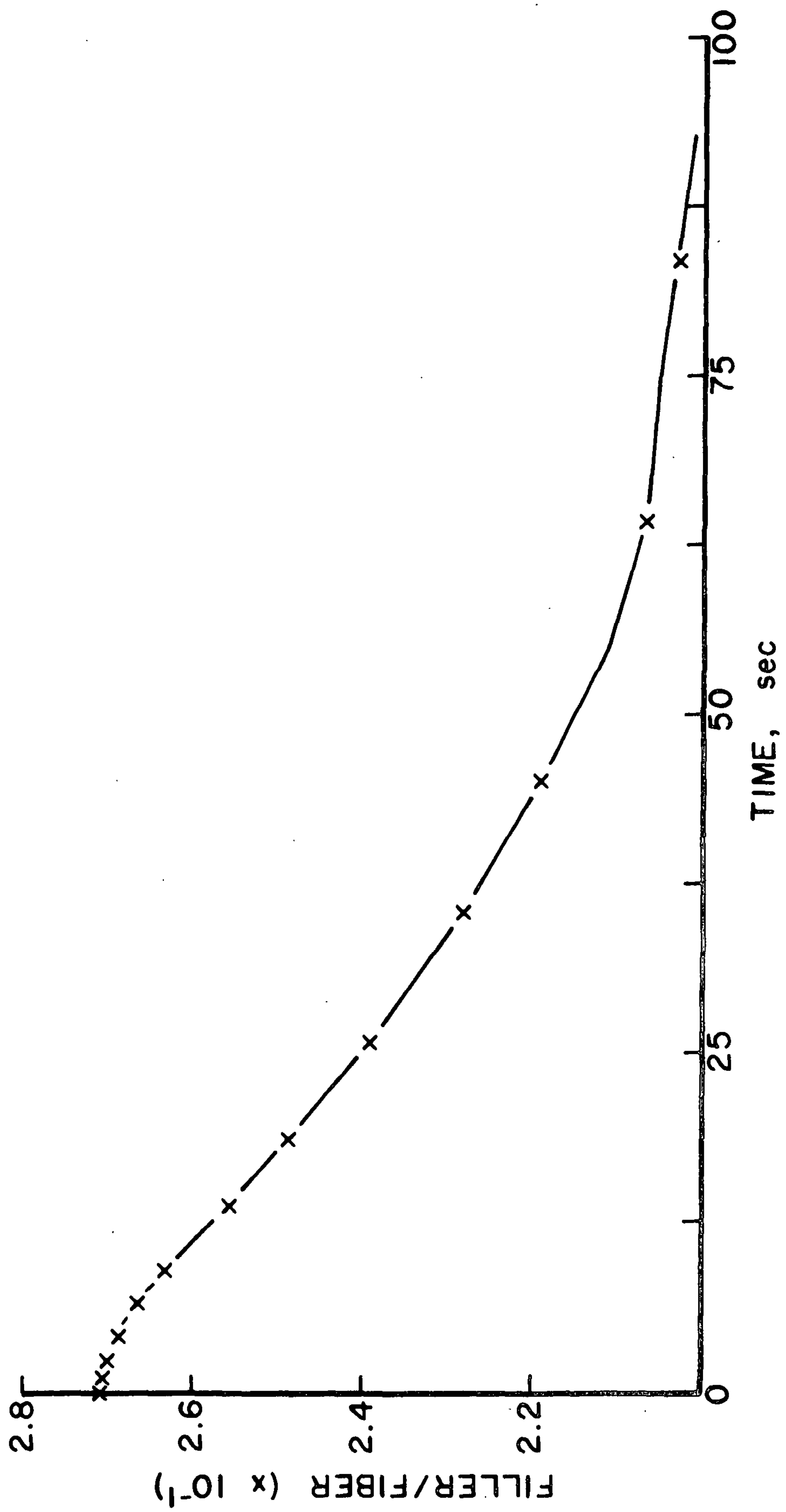

Figure 7. Option No. 4 - Fiber/Filler Ratio at Saveall Input

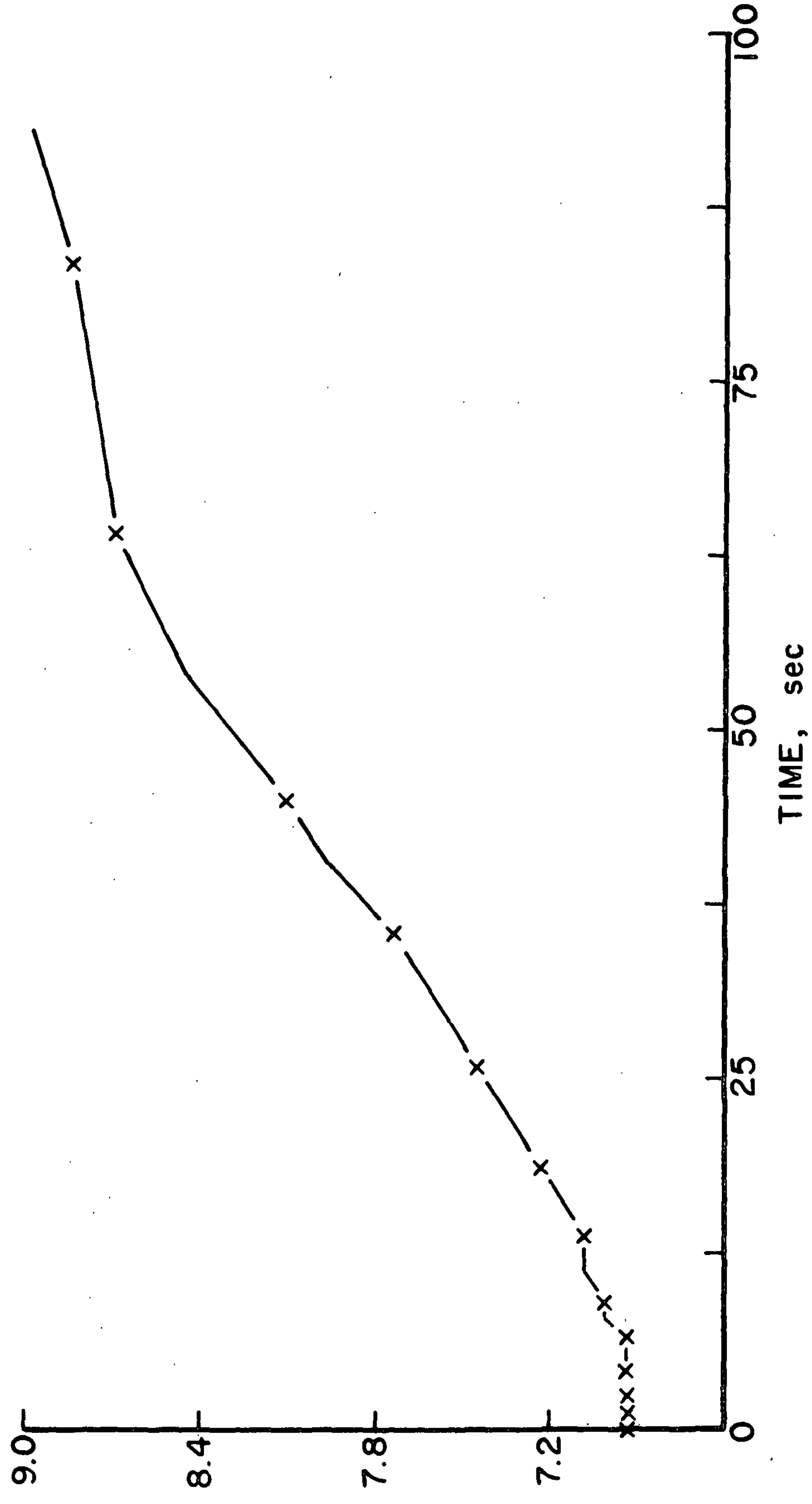

Figure 8. Option No. 4 - Filler/Fiber Ratio for Cloudy Filtrate

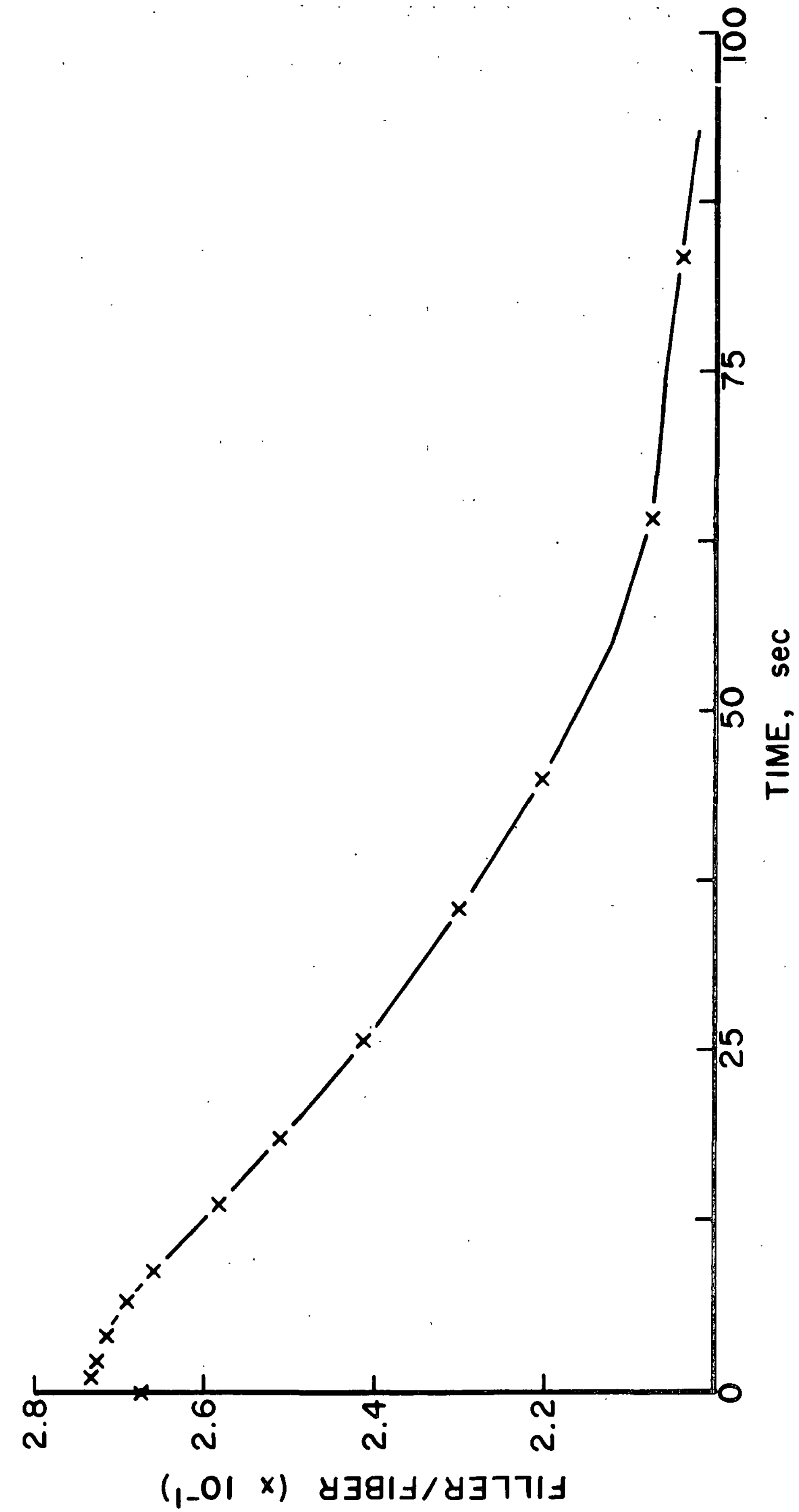

Figure 9. Option No. 4 - Filler/Fiber Ratio for Saveall Cake

was formulated. This problem is a typical screen room which involves 6 fiber fractions, water and steam. The basic flow sheet is given in Fig. 10, while Fig. 11 is the corresponding simulation block diagram. Table VII lists the various specifications for the problem.

One of the purposes of this problem was to evaluate the ease with which new models could be added to the simulation package. Thus, various specifications were put on the model. The model equations are given in Table VIII.

DYSCO was not included in the official TAPPI comparison studies as it is not classed as a steady state simulator. Since it solves steady state problems as well as dynamic problem, we decided to do this simulation. Four new process models were required. In addition, this simulation required that the steam physical properties package be implemented. All of these tasks were relatively easy to do and greatly increase the utility of DYSCO.

Table IX presents a summary of the results of this study. The mass balance closes, as expected. In other words, the steady state results fall within he criteria specified by the user. In addition, all stream flows agree with the steady state flows of the simulators used in this comparison test (9).

This problem showed how easily process models can be added to the simulator library. In addition, it demonstrated that while DYSCO is truly a dynamic simulator, it is also capable of solving steady state problems. In fact, this exercise has convinced us to add some additional models for steady state convergence acceleration to give DYSCO a strong steady state capability in addition to its dynamic capability. This problem also demonstrated the ease with which the physical properties package can be expanded.

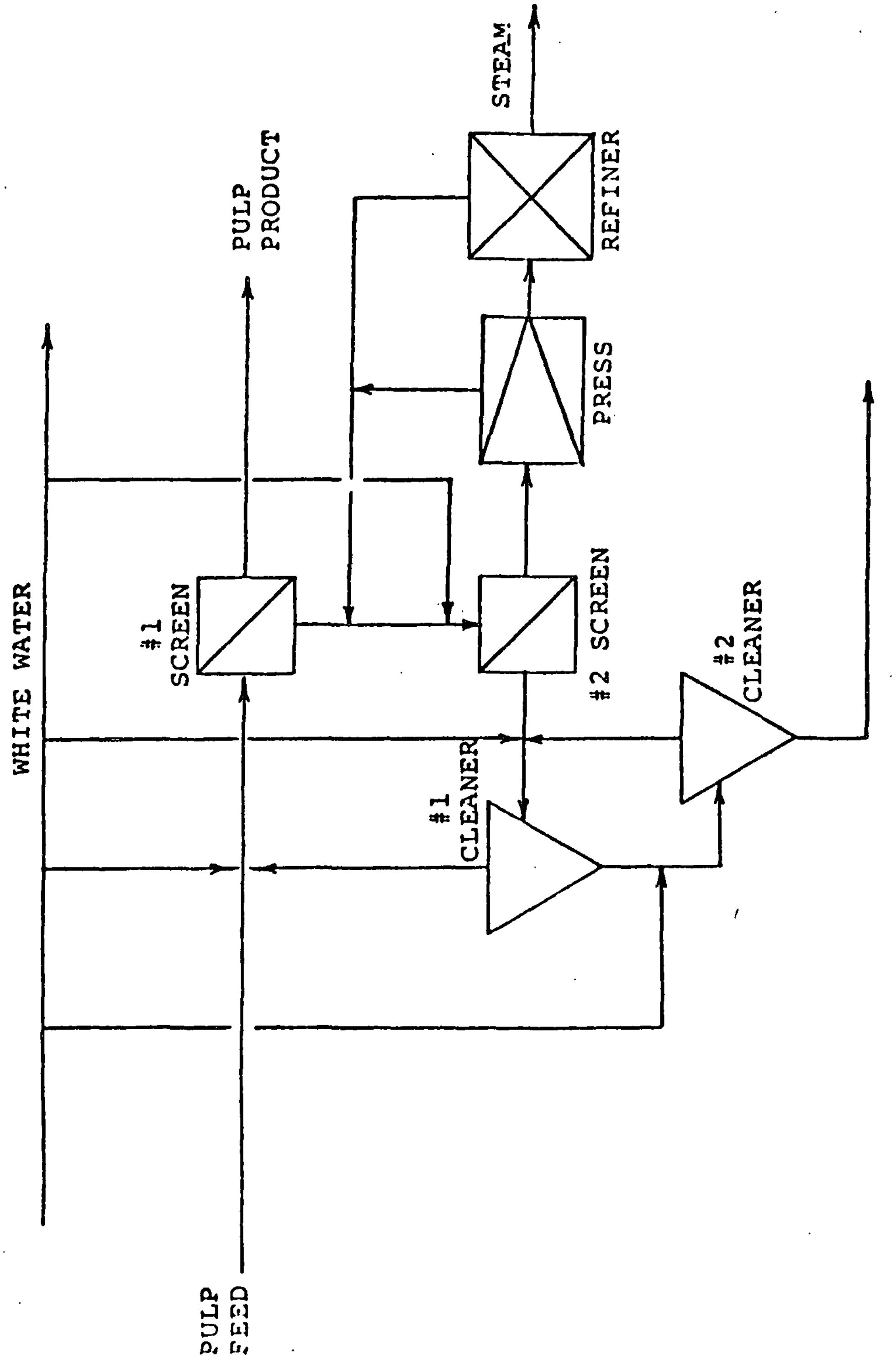

Figure 10. Process Diagram - TAPPI Benchmark Problem

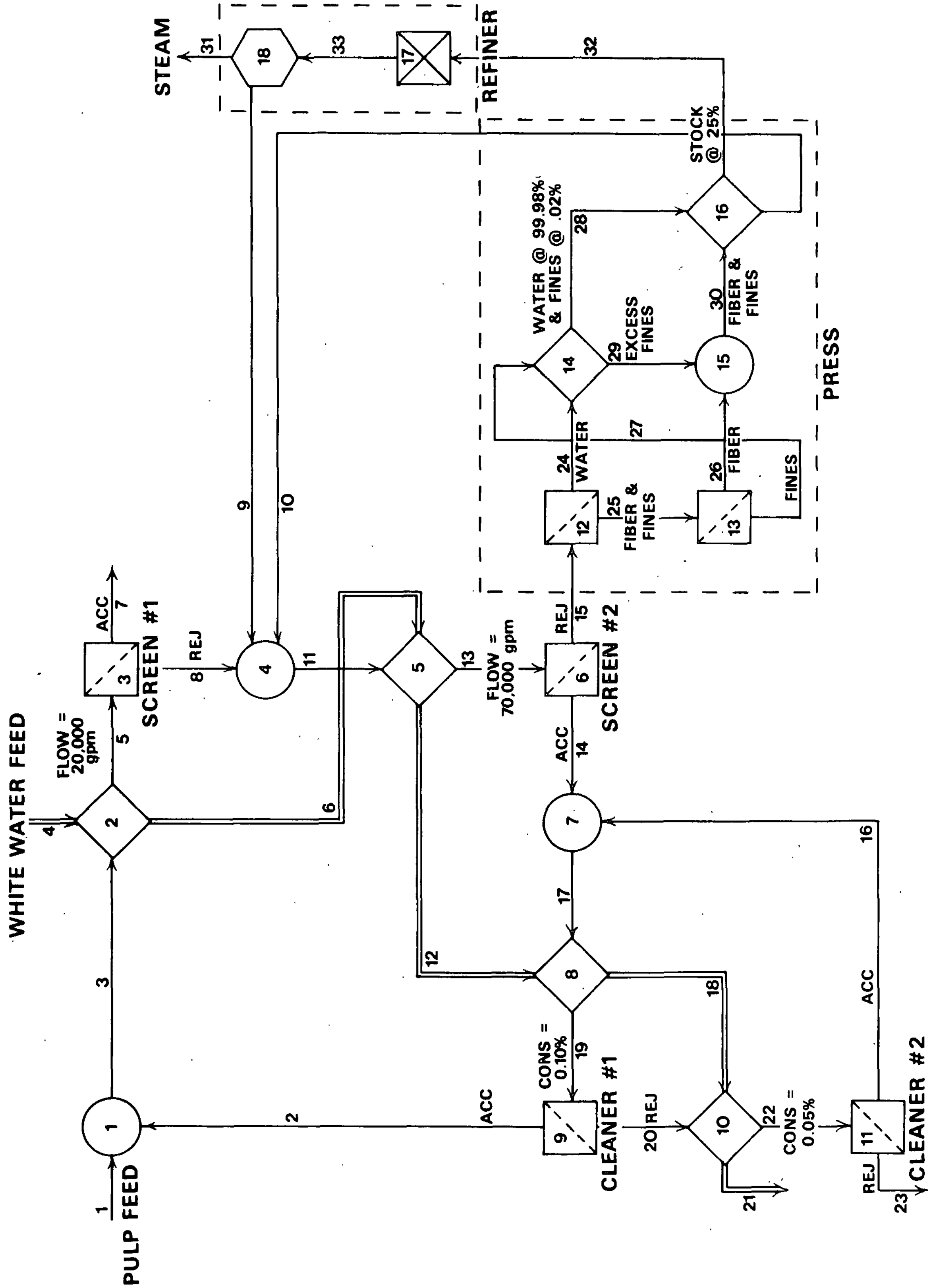

Figure 11. Simulation Diagram - Benchmark Problem

TABLE VII

TAPPI BENCHMARK PROBLEM SPECIFICATIONS

Inputs:

Feed:

Fiber fraction	Rate, tons/day
P100	250
48/100	250
28/48	200
14/28	80
R14	30
Shives	8
Consistency	3.25%
Temperature	135°F

White Water:

P100	0.02 weight %
Water	99.98 weight %
Temperature	140°F

Screen No. 1

Inlet flow	70,000 GPM
Reject ratio	16%

Screen No. 2

Inlet Flow	20,000 GPM
Reject ratio	16%

TABLE VII (continued)

TAPPI BENCHMARK PROBLEM SPECIFICATIONS

Cleaner No. 1	
Inlet consistency	0.10%
Reject ratio	5%
Cleaner No. 2	
Inlet consistency	0.05%
Reject ratio	4.5%
Press:	
White water consistency (P100 fraction only)	0.02%
Thick stock consistency	25%
Refiner:	
Specific horsepower	55 hp-day/ton

TABLE VIII

TAPPI BENCHMARK PROBLEM MODELS

Cleaner/Screen

$$E_{r_i} = \frac{Rv}{1 - Q_i\ (1-Rv)}$$

where:

$$E_{r_i} = \frac{\text{mass of fiber fraction i in rejects}}{\text{mass of fiber fraction i in feed}}$$

$$Rv = \text{reject ratio} = \frac{\text{volume flow of rejects}}{\text{volume flow of feed}}$$

Q_i = constant for each fraction

Fraction	Q_i
P100	-0.30
48/100	0.00
28/48	0.30
14/28	0.55
R14	0.80
Shives	0.95

Cleaner and screen are isothermal

Refiner

$$\text{Log } (1-R_i) = -A_i \cdot SP$$

$$R_i = \frac{f_i^{\,i} - f_o^{\,i}}{f_i^{\,i}}$$

TABLE VII (continued)

TAPPI BENCHMARK PROBLEM MODELS

f_i^i = mass of fiber fraction i in inlet

f_o^i = mass of fiber fraction i in outlet

A_i = a constant for each fraction

sp = refiner specific horsepower in hp-day-ton

Fraction	A_i
P100	--
48/100	0.00
28/48	0.0027
14/28	0.0055
R14	0.0095
Shives	0.0161

Total mechanical energy is adsorbed as heat and steam is vented.

In essence, the refiner converts mechanical energy to heat. The P100 fraction collects fines from the refining of the other fractions and is used to insure that the fiber mass balance is satisfied.

TABLE IX

RESULTS OF TAPPI BENCHMARK SIMULATION

** STREAM FLOWS AND COMPOSITIONS

STRM NO	T (C)	P PSIA	FLOW #/MIN	WATER	P100	48/100	28/48	14/24
				R14	SHIVES			
1	57.2	14.7	34957	0.967820	0.009933	0.009933	0.007946	0.003178
				0.001192	0.000318			
2	59.4	14.7	345476	0.999019	0.000438	0.000191	0.000198	0.000103
				0.000047	0.000004			
3	59.2	14.7	380428	0.996152	0.001311	0.001086	0.000910	0.000386
				0.000152	0.000033			
4	59.4	14.7	1000000	0.999800	0.000200	0.000000	0.000000	0.000000
				0.000000	0.000000			
5	59.3	14.7	583800	0.997423	0.000924	0.000708	0.000593	0.000251
				0.000099	0.000022			
6	59.4	14.7	796628	0.999800	0.000200	0.000000	0.000000	0.000000
				0.000000	0.000000			
7	59.3	14.7	490392	0.997525	0.000959	0.000708	0.000555	0.000210
				0.000060	0.000005			
8	59.3	14.7	93408	0.996886	0.000738	0.000708	0.000792	0.000467
				0.000302	0.000107			
9	100.0	14.7	207	0.602945	0.206894	0.060722	0.063964	0.036604
				0.023318	0.005554			
10	59.4	14.7	26358	0.999800	0.000200	0.000000	0.000000	0.000000
				0.000000	0.000000			
11	59.3	14.7	119974	0.996845	0.000976	0.000656	0.000728	0.000427
				0.000275	0.000093			
12	59.4	14.7	749802	0.999800	0.000200	0.000000	0.000000	0.000000
				0.000000	0.000000			
13	59.4	14.7	166800	0.997675	0.000758	0.000472	0.000523	0.000307
				0.000198	0.000067			
14	59.4	14.7	140112	0.997857	0.000787	0.000472	0.000490	0.000257
				0.000121	0.000017			

TABLE IX (continued)

RESULTS OF TAPPI BENCHMARK SIMULATION

15	59.4	14.7	26688	0.996717	0.000606	0.000472	0.000700	0.000571	0.000603	0.000332
16	59.4	14.7	67227	0.999522	0.000238	0.000049	0.000072	0.000056	0.000051	0.000012
17	59.4	14.7	207337	0.998397	0.000609	0.000335	0.000354	0.000192	0.000098	0.000015
18	59.4	14.7	593481	0.999800	0.000200	0.000000	0.000000	0.000000	0.000000	0.000000
19	59.4	14.7	363659	0.999000	0.000433	0.000191	0.000202	0.000109	0.000056	0.000009
20	59.4	14.7	18183	0.998639	0.000337	0.000191	0.000282	0.000229	0.000233	0.000089
21	59.4	14.7	541269	0.999800	0.000200	0.000000	0.000000	0.000000	0.000000	0.000000
22	59.4	14.7	70394	0.999500	0.000235	0.000049	0.000073	0.000059	0.000060	0.000023
23	59.4	14.7	3167	0.999038	0.000183	0.000049	0.000102	0.000125	0.000255	0.000248
24	59.4	14.7	26600	1.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
25	59.4	14.7	87	0.000000	0.184470	0.143728	0.213123	0.173869	0.183819	0.100990
26	59.4	14.7	71	0.000000	0.000000	0.176239	0.261331	0.213198	0.225398	0.123834
27	59.4	14.7	16	0.000000	1.000000	0.000000	0.000000	0.000000	0.000000	0.000000
28	59.4	14.7	26605	0.999800	0.000200	0.000000	0.000000	0.000000	0.000000	0.000000
29	59.4	14.7	10	0.000000	1.000000	0.000000	0.000000	0.000000	0.000000	0.000000
30	59.4	14.7	82	0.000000	0.131734	0.153022	0.226905	0.185113	0.195705	0.107521
31	100.0	14.7	122	1.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
32	59.4	14.7	329	0.750000	0.033064	0.038233	0.056692	0.046250	0.048897	0.026864
33	339.7	14.7	329	0.750000	0.130268	0.038233	0.040274	0.023047	0.014682	0.003497

III. ACTIVATED SLUDGE PLANT SIMULATION MODEL

Closure of pulp and paper mill water systems decreases the average flow to the waste treatment plant. The concentration of dissolved and suspended components will normally increase. As the normal process water consumption decreases, intermittent losses, such as spills, can contribute a greater fraction to the instantaneous flow than under more open conditions.

Thus, the treatment facility for a mill with a highly closed water system may experience stronger and wider fluctuations in the quantity and quality of the plant influent. Unfortunately, biological processes can be seriously upset by such fluctuations and performance may suffer for some time before the process returns to the normal state.

Treatment plants must be protected from some fluctuations, but the design of an equalization basin or spill containment system should be sized after considering the expected variations and determination of what degree of variability the plant can accommodate. Modelling can help answer some of these questions.

Another impetus for detailed modelling of the waste treatment plant is that good process control systems have the potential of improving plant performance. Thus, it may be possible to meet more stringent guidelines by improved control. Models that include an estimation of process kinetics provide a starting point for developing new and/or improved control schemes.

There has been a great deal of work done in modelling waste treatment processes. Excellent reviews are those by Lawrence and McCarty (10), Andrews (11), Saunders (12) and Ekama and V. R. Marais (13,14). The basis for our biological reactor model is the work of Busby (4). We have extended his model to include two types of organisms and have included an arbitrary toxicity function which retards organism growth. The modified model has been included as a process model in the DYSCO library.

A description of the model follows:

Let:

F = Volumetric feed rate

X_1 = Concentration of live, type 1 organisms

X_2 = Concentration of live, type 2 organisms

X_3 = Concentration of dead (inactive), type 1 organisms

X_4 = Concentration of dead type 2 organisms

X_5 = Concentration of dissolved oxygen

X_6 = Concentration of dissolved, biologically oxidizable material

X_7 = Concentration of suspended, biologically oxidizable material

X_8 = Concentration of dissolved, nonoxidizable material

X_9 = Concentration of suspended, nonoxidizable material

X_{10} = Concentration of potential toxic, biologically oxidizable material

V = Volume of the reactor; assumed constant

b_1, b_2 = Endogenous respiration coefficients for type 1 and 2 organisms

d_1, d_2 = Death rate constants for type 1 and 2 organisms

K_1, K_2 = Half saturation constants for organism 1 and 2

K_3, K_4 = Rate constants for lysis for organism 1 and 2

T_1, T_2 = Toxicity factors for organism 1 and 2

Y_1, Y_2 = Yield coefficients for type 1 and 2 organisms

α_1, α_2 = Stoichiometric coefficient for oxygen utilized in growth

β_1, β_2 = Stoichiometric coefficient for oxygen utilized in respiration

γ_6, δ_6 = Fraction of dead organism 1 or 2 that becomes soluble and oxidizable

γ_7, δ_7 = Fraction of dead organism 1 or 2 that becomes suspended and oxidizable

γ_8, δ_8 = Fraction of dead organism 1 or 2 that becomes soluble and nonoxidizable

γ_9, δ_9 = Fraction of dead organism 1 or 2 that becomes suspended and nonoxidizable

i = Subscript for ith input stream

o = Subscript for oth output stream

A mass balance for an organism yields:

$$V \frac{dX_1}{dt} = \sum_i F_i X_{1_i} - X_1 \sum_o F_o \qquad : \text{ net flow}$$

$$+ \frac{\mu_1 (X_6 + X_7 + X_{10})}{k_1 + (X_6 + X_7 + X_{10})} \cdot X_1 \cdot V \cdot T_1 \qquad : \text{ growth}$$

$$- Vb_1X_1 \qquad : \text{ respiration}$$

$$- Vd_1 X_1 \qquad : \text{ death}$$

with a similar equation for organism type 2.

For dead organisms:

$$V \frac{dX_3}{dt} = \sum_i F_i X_{3_i} - X_3 \sum_o F_o \qquad : \text{ net flow}$$

$$+ Vd_1X_1 \qquad : \text{ from death of } X_1$$

$$- Vk_3X_3 \qquad : \text{ lysis}$$

and a similar equation holds for type 2 dead organisms

A dissolved oxygen balance yields:

$$V \frac{dX_5}{dt} = \sum_i F_i X_{5_i} - X_5 \sum_o F_o \qquad : \text{ net flow}$$

$$+ R_A \qquad : \text{ aeration}$$

$$-\alpha_1 \frac{\mu_1 (X_6 + X_7 + X_{10})}{k_1 (X_6 + X_7 + X_{10})} \cdot X_1 \cdot V \cdot T_1 \qquad : \text{ } O_2 \text{ for growth}$$

$$-\alpha_2 \frac{\mu_2 (X_6 + X_7 + X_{10})}{k_2 + (X_6 + X_7 + X_{10})} \cdot X_2 \cdot V \cdot T_2 \qquad : \text{ } O_2 \text{ for growth}$$

$$-\beta_1 V b_1 X_1 \qquad : \text{ respiration}$$

$$-\beta_2 V b_2 X_2 \qquad : \text{ respiration}$$

The material balances for oxidizable substances are:

$$V \frac{dX_6}{dt} = \sum_i F_i X_{6_i} - X_6 \sum_o F_o \qquad : \text{ net flow}$$

$$- \frac{1}{Y_1} \cdot \frac{\mu_1 (X_6)}{K_1 + (X_6 + X_7 + X_{10})} \cdot V \cdot X \cdot T \qquad : \text{ organism growth}$$

$$- \frac{1}{Y_2} \cdot \frac{\mu_2 (X_6)}{K_2 + (X_6 + X_7 + X_{10})} \cdot V \cdot X_2 \cdot T_2 \qquad : \text{ organism growth}$$

$$+ \gamma_6 V k_3 X_3 \qquad : \text{ from lysis}$$

$$+ \delta_6 V k_4 X_4 \qquad : \text{ from lysis}$$

$$V \frac{dX_7}{dt} = \sum_i F_i X_i - X_7 \sum_o F_o \qquad : \text{ net flow}$$

$$- \frac{1}{Y_1} \frac{\mu_1 (X_7)}{K_1 + (X_6 + X_7 + X_{10})} \cdot X_1 \cdot V \cdot T_1 \qquad : \text{ organism growth}$$

$$- \frac{1}{Y_2} \frac{\mu_2 (X_7)}{K_2 + (X_6 + X_7 + X_{10})} \cdot X_2 \cdot V \cdot T_2 \qquad : \text{ organism growth}$$

$$+ \gamma_7 V k_3 X_3 \qquad : \text{ from lysis}$$

$$+ \delta_7 V k_4 X_4 \qquad : \text{ from lysis}$$

The nonoxidizable components material balances are simpler as they do not contain loss terms due to organism growth:

$$V \frac{dX_8}{dt} = \sum_i F_i X_{8_i} - X_8 \sum_o F_o \qquad : \text{ net flow}$$

$$+ \gamma_8 V k_3 X_3 + \delta_8 V k_4 x_4 \qquad : \text{ from lysis}$$

$$V \frac{dX_9}{dt} = + \sum_i F_i X_{9_i} - X_9 \sum_o F_o \qquad : \text{ net flow}$$

$$+ \gamma_9 V k_3 X_3 + \delta_9 V k_4 X_4 \qquad : \text{ from lysis}$$

The balance for the toxic material is similar to that for the other dissolved, oxidizable components:

$$V \frac{dX_{10}}{dt} = \sum_i F_i X_{10_i} - X_{10} \sum_o F_o \qquad : \text{ net flow}$$

$$-\frac{1}{Y_1}\,\frac{\mu_1\,(X_{10})}{K_1 + (X_6 + X_7 + X_{10})} \cdot X \cdot V \cdot T \qquad : \text{ organism growth}$$

$$-\frac{1}{Y_2}\,\frac{\mu_2\,(X_{10})}{K_2 + (X_6 + X_7 + X_{10})} \cdot X \cdot V \cdot T \qquad : \text{ organism growth}$$

Unfortunately, the majority of the constants are either not measurable or measurable only with extreme difficulty. The toxicity factor, T_1 or T_2, is a novel idea and was incorporated to allow us to estimate treatment plant behavior under shock loadings of toxic materials. The basic form for this factor is given in Fig. 12. The user of the model defines the two limits, C_L and C_U, for the toxicity function. If the concentration is below C_L, the function has a value of 1 and the toxic component acts as an additional food source to the biological reactor's organisms; there is no influence on the growth rate. Above C_U, the toxicity factor is 0 and effectively stops organism growth. Between C_L and C_U, the toxic component serves both as a food source and as a growth retarding agent. Mathematically, the function in Fig. 12 is:

$$T = \begin{cases} 0 & C \geq C_U \\ \dfrac{C_U - C}{C_U - C_L} & C < C < C \\ 1 & C \leq C_L \end{cases}$$

As mentioned previously, many of the constants in the model are difficult or nearly impossible to measure. In addition, the model does not compute terms familiar to most treatment plant analysts. That is, such terms as mixed liquor volatile suspended solids (MLVSS), BOD, etc. must be computed from the model. Some of these terms are relatively easy to calculate. For example:

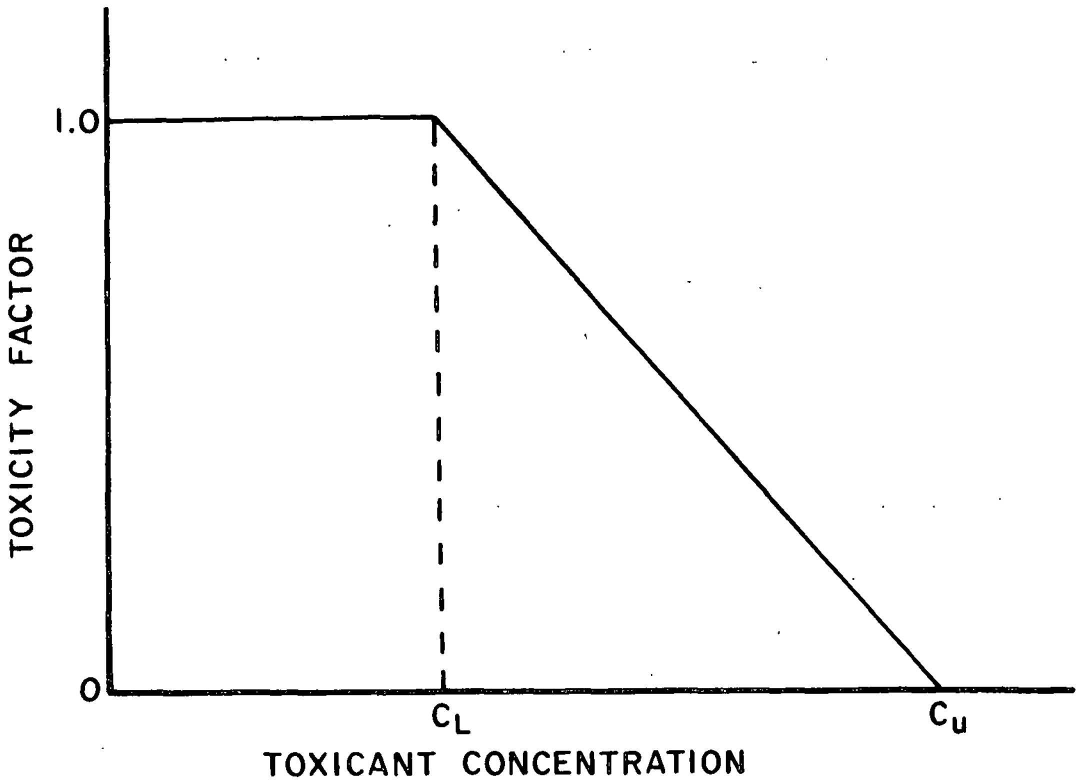

Figure 12. Toxicant Factor

$$MLVSS = X_1 + X_2 + X_3 + X_4 + X_7$$

$$MLSS = MLVSS + X_9$$

The food source for the organisms could be measured as BOD, COD, TOC, or some other measure of food availability. The important consideration is that growth rate constants and yield coefficients are consistent with the form of organic substrate measure.

To test the model, a series of laboratory activated sludge reactors were run. The feed stream was a BOD standard solution of glucose/glutamic acid plus necessary nutrients. The experiments were set up and the data analyzed according to methods outlined in Ramahlo (15). Analysis of the experimental data gives values for the coefficient: μ/K, Y, b, α, and β (Table X).

TABLE X

EXPERIMENTAL ACTIVATED SLUDGE MODEL PARAMETERS

μ/K	=	0.143 day^{-1}
Y	=	0.428 mg MLVSS/mg BOD removed
b	=	0.055 day^{-1}
α	=	0.549 mg O_2/mg BOD removed
β	=	0.491 mg O_2/mg MLVSS

The laboratory system was simulated by using the experimental coefficients plus literature estimates in the model. Figure 13 and 14 are the predicted MLVSS and effluent BOD from the model. These predictions, although not identical, compare well with the measured data.

The impact of an input spike of a toxic compound was simulated. In this experiment, the reactor was initially populated by two organisms with identical biological behavior except their response to the toxicant. Figure 15 shows the two responses to the toxicant; organism 2 is much more tolerant. The input spike is shown in Fig. 16 and the system responses are shown in Fig. 17-19. The BOD (Fig. 17) first rises, then falls to its initial level as toxicant is degraded and washed out of the system. The relative ratio of the organisms also shifts (Fig. 18), as type 1 organisms are at a competitive disadvantage. The toxicant (Fig. 19) concentration responds as expected. Note that although the spike was only of 4 hours duration, it took over 20 hours for the reactor to again reach a steady state.

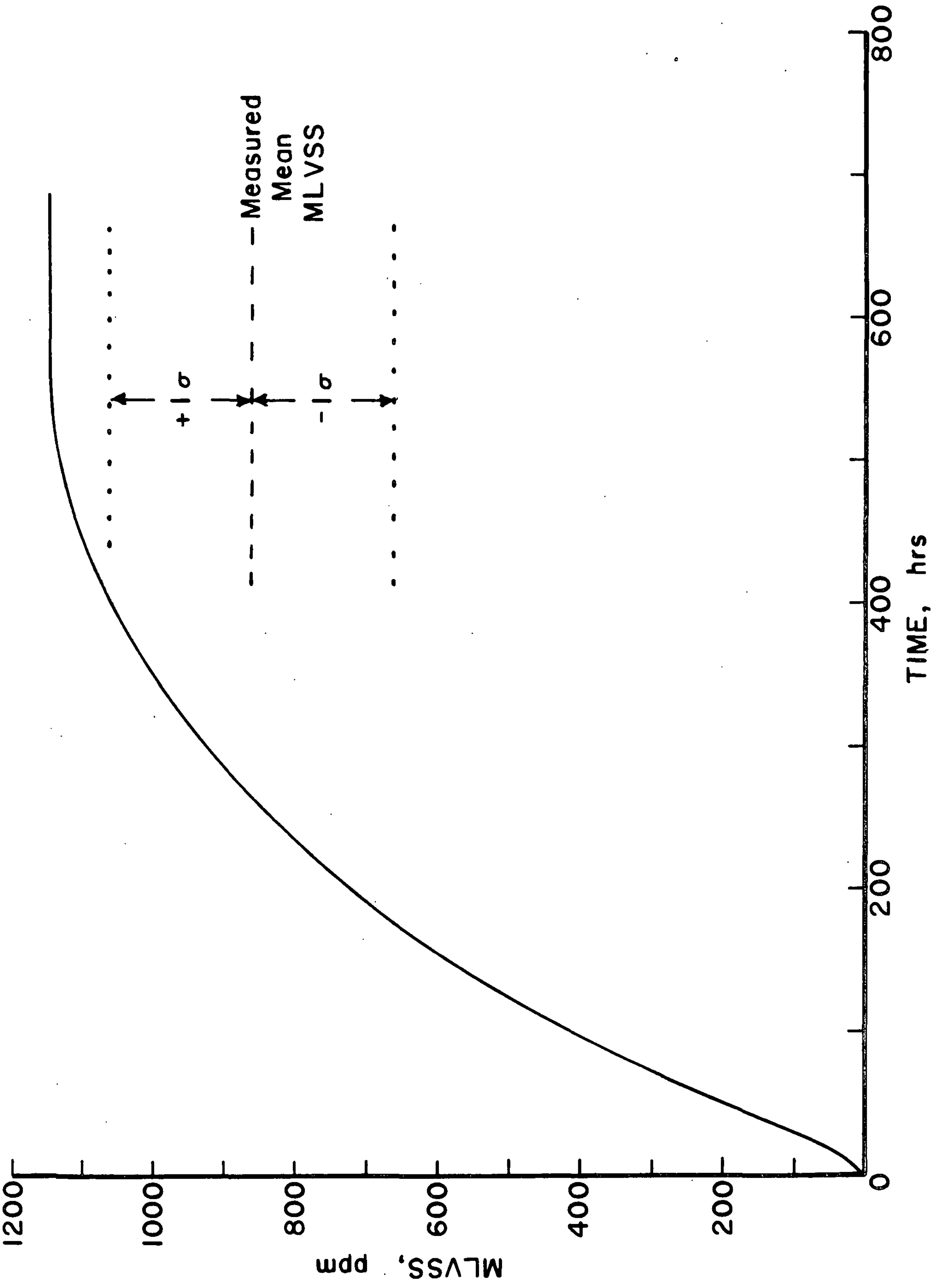

Figure 13. Biological Reactor Dynamics

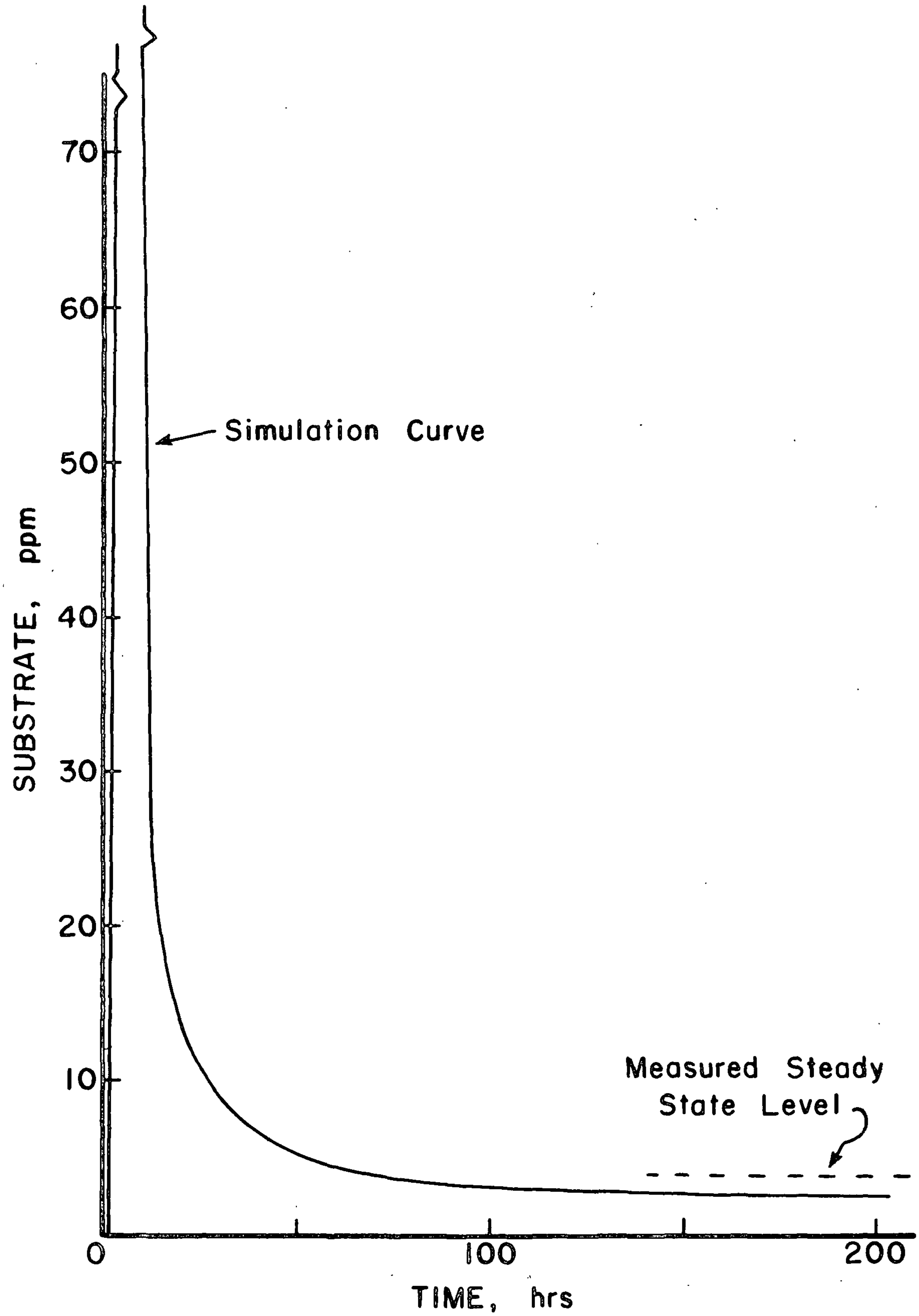

Figure 14. Substrate Removal

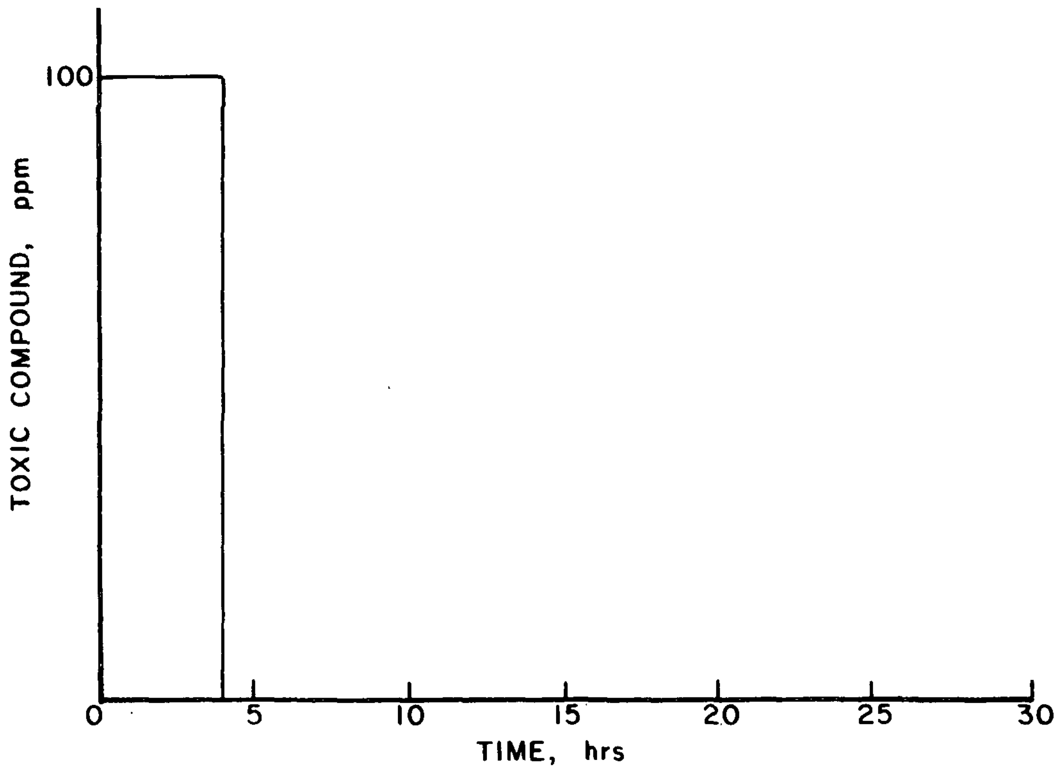

Figure 15. Toxicity Factor for Simulation Run

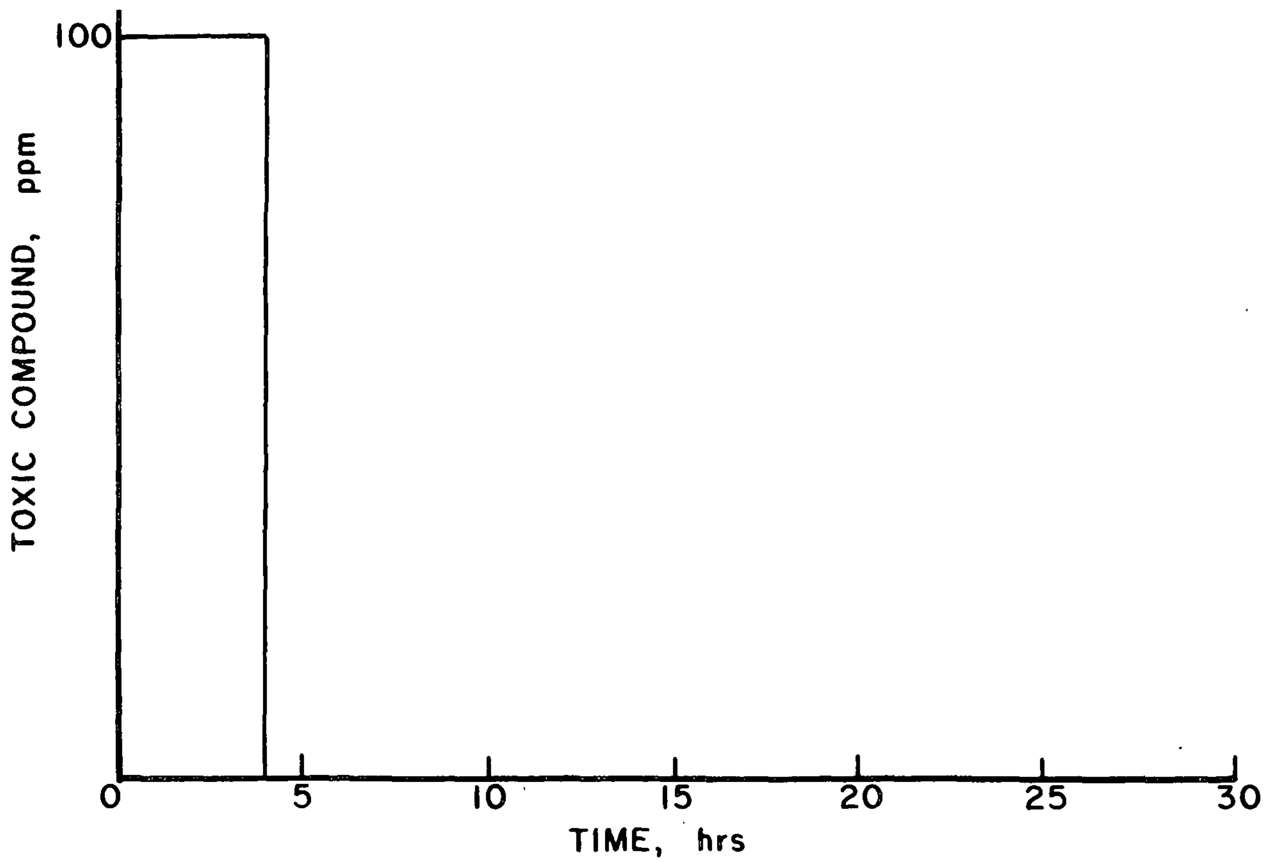

Figure 16. Toxic Spike

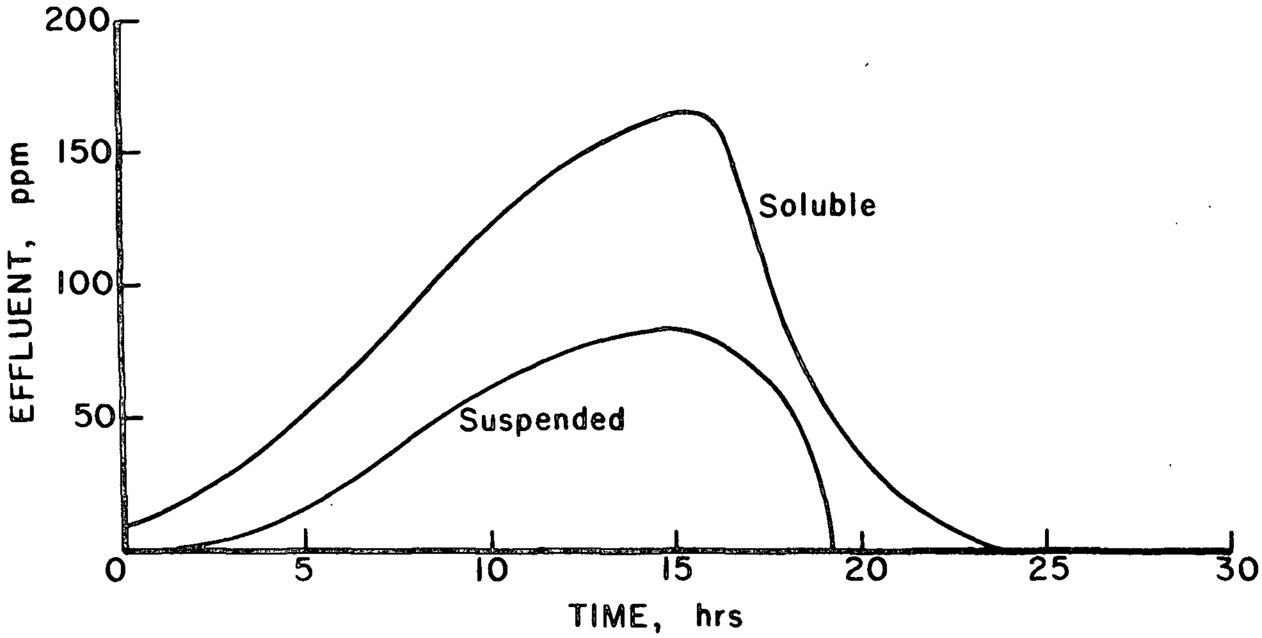

Figure 17. Effluent BOD

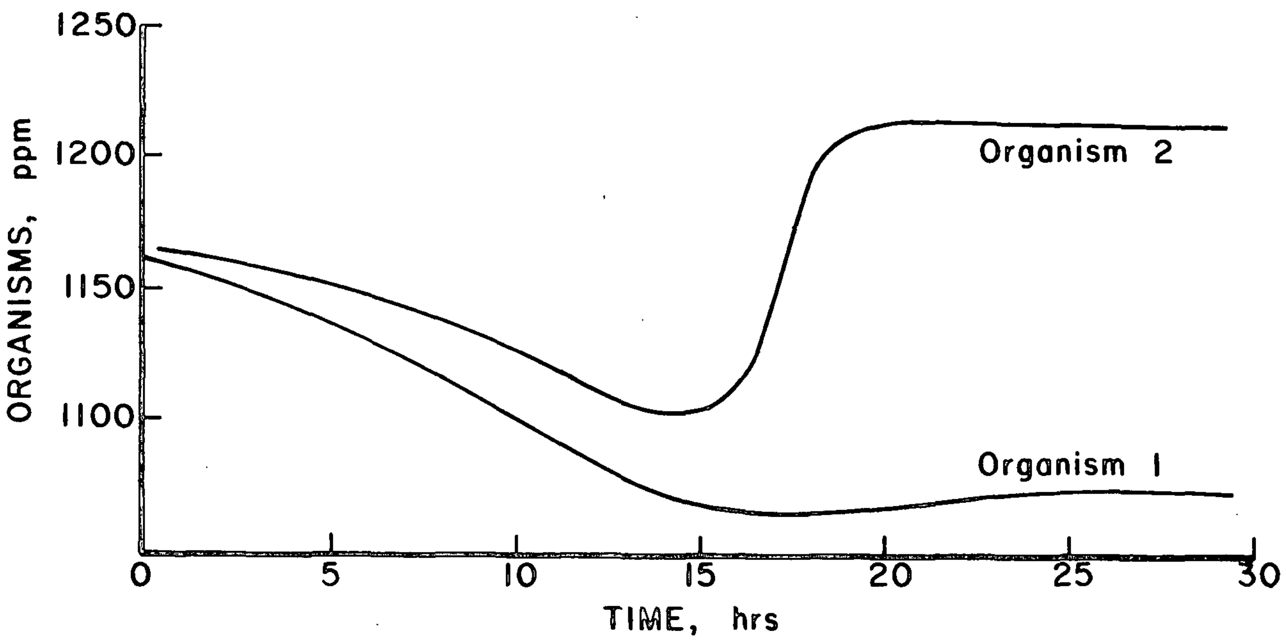

Figure 18. Reactor Population

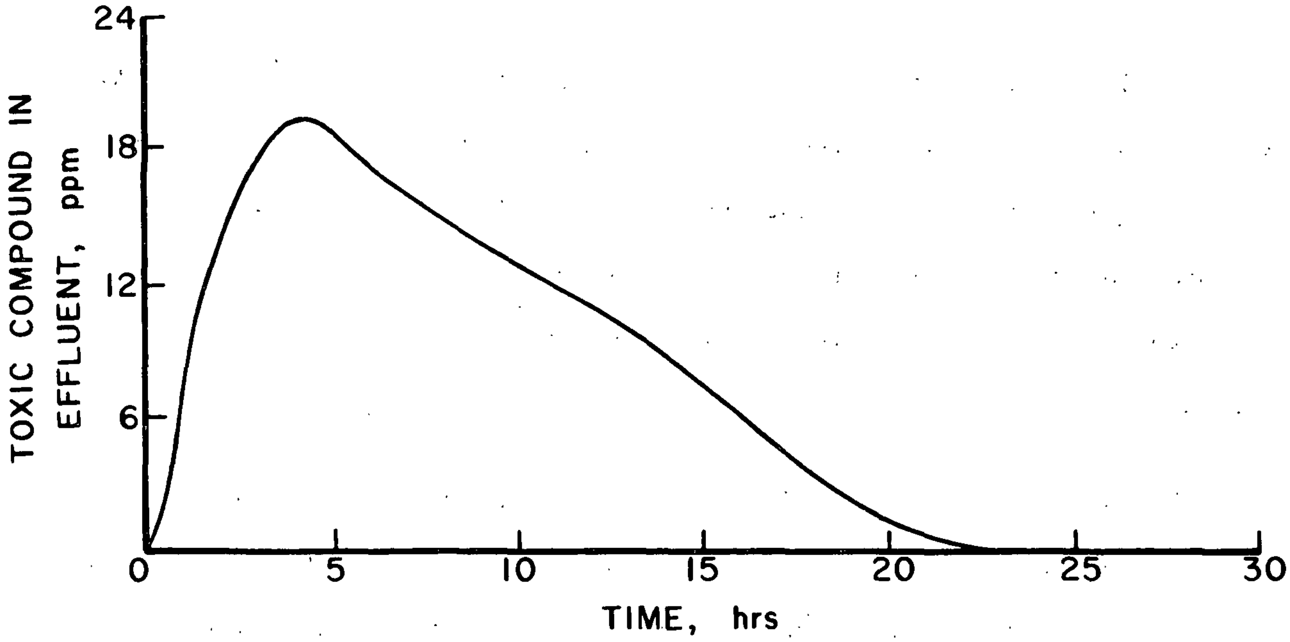

Figure 19. Toxic Component in Effluent

CONCLUSIONS

DYSCO has proven to be a very versatile, easy-to-use simulation package. The addition of new models and the extension of the physical properties package has proven to be quite simple. The paper machine modelling effort has shown that both dynamic and steady state simulations can easily be done with the same simulator. Both the steady state and dynamic solutions to simulator problems are valuable in investigating a process.

The addition of a nontraditional process, the activated sludge plant, demonstrated the versatility of the simulator. The ability of this model to predict the behavior of laboratory activated sludge systems shows that it holds promise for future waste treatment plant control studies.

FUTURE WORK

Necessary future work should be focused in four areas:

- The Simulator
- Physical Properties
- Process Models
- Waste Treatment Models

The simulator itself needs some work. In particular, some changes should be made to make it a more efficient steady state simulator. In addition, some changes should be incorporated so that all steady state process loops are converged at each time step of a dynamic simulaton. Long range planning should include the incorporation of a stiff differential equation solving routine or routines.

The physical properties package needs much development and should be a long-term, low level effort task. As needs for properties become apparent, they should be incorporated. DYSCO is structured such that expansion of this package should be relatively easy. The more data that are available as physical properties, the more accurate the simulation will be.

The process model library is the mainstay of the simulator package. At the present, only relatively simple process models are incorporated into the library. These are primarily for the papermaking process. The work of Sklarewitz (6) should be verified to allow incorporation of the bleach plant models. Additional work in modelling other areas of the pulping and papermaking process is needed.

The biological reactor model needs extensive testing before it should be included in the DYSCO library. In particular, a real facility should be accurately simulated before the model is accepted as representing the real world.

Other waste treatment operations should be considered for study. The primary and secondary clarifiers need to be adequately modelled before a conventional activated sludge process can be realistically modelled. Other methods of treatment, such as aerated stabilization basins or lagoons need to be studied. The current biological reactor model should serve as the basis for these later models, as biological reactions should be similar. The inclusion of anerobic decomposition will be a necessary extension.

The above future work areas would occupy several people for several years. Priorities and effort levels will be set through projection of industry needs and in consultation with industry advisory groups.

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